Compact QIT-Mass Spectrometer for Lunar and Planetary Applications

389Team Planetary Mass Spectrometry

Frank Maiwald, 389T Group Supervisor
Stojan Madsunkov (Technical Lead), Dragan Nikolic, Jurij Simcic, Richard Kidd, Marianne Gonzalez, Anton Belousov, Byunghoon Bae, Max Coleman, Valeria Lopez, Bohoon Kim

National Aeronautics and Space Administration
Jet Propulsion Laboratory
California Institute of Technology

Areas of Interest

- Introduction of Mass Spectrometry Team at JPL
- Past and recent Developments
- Component Developments
  - S.A.M. Spacecraft Atmosphere Monitor
  - Concepts
  - Compact QIT-Mass Spectrometer
- Publications
- Past Proposals
- Science
  - Performance driver
  - Noble Gases
  - High resolution
- Conclusions
- Future Roadmap
- Discussions

Meet the Core 389Team

Dr. Frank Maiwald

Dr. Stojan Madzunkov

Dr. Jurij Semcic

Dr. Dragan Nicolic

Dr. Richard Kidd

Dr. Anton Belousov

Dr. Byunghoon Bae

Marianne Gonzalez

Dr. Max. Coleman

Typical Education
- Physics
- Chemistry
- Electronics
- Geoscience

Valeria Lopez

Dr. Bohoon Kim

Experience
- Physics and Chemistry
- Theory and modelling
- Instrument development
- Publications and proposals
- Teamwork

Goals of the 389Team

- The **Planetary Mass Spectrometry Group 389T** is developing the QIT-MS for space applications with the goal to explore the solar system by in-situ measurements of chemical compositions and isotopic ratios.
  - Capabilities:
    - Development of components and instruments based on **QIT-MS** for Earth and space applications.
  - Expertise:
    - Mass spectrometer and subsystem components, including electronics and science software
    - Expertise in stable isotope geochemistry, planetology, sedimentology, forensic science, Earth Science
  - Additional fields of expertise include:
    - **Radiation Shielding Experiment (RSE):** To simulate and verify an effective electrostatic shield by experiment in the laboratory and finally with a shielding demonstrator in space.
    - **Life Detection and Assessment of Habitability (LDAH):** To detect biosignatures for life detection with mass spectrometry, action spectroscopy (in early stage), or IR Capillary Absorption Spectrometry (Methane and water isotopes projects in progress)

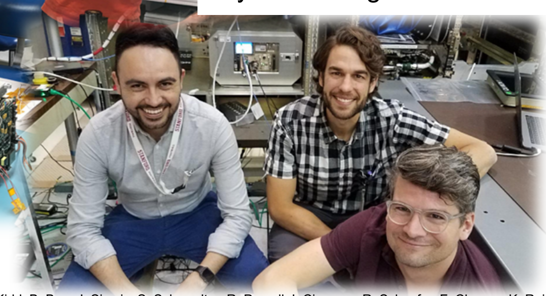
Instrument Development and Applications

- NASA instrument and JPL strategic funding for:
  - GC-QIT-MS for trace species detection for ISS cabin heath monitoring
    - VCAM and S.A.M.
  - ESI-QIT-MS for exploring ocean worlds
- QIT-MS with applications driven by sample input
  - Significant reduction in mass, power, volume, and data rate over past decade
  - Focus on TRL enhancement for flight applications and transition to commercialization

Members of the Vehicle Cabin Atmosphere Monitor team, from left: Ara Chutjian, Dan Karmon, Jim Hofman, Benny Toomarian, Murray Darrach, John MacAskill, Stojan Madzunkov, Arvid Croonquist and Richard Kidd.

MCA (Major Constituent Analysis) with 2 sec updates and fraction of a percent error (performance checkout underway)

TGA (Trace Gas Analysis) with daily 20 minutes runs, down to 10-1000ppb Dynamic range 10^0 to 10^{-8}



M. Darrach, S. Madzunkov, E. Diaz, B. Moore, R. Kidd, B. Bae, J. Simcic, S. Schowalter, R. Purcell, I. Cisneros, R. Schaefer, F. Cheung, K. Reichenbach, T. Loc, J. Lam, A. Oyake, D. Nikolic, R. murdock

Vehicle Cabin Atmosphere Monitor (VCAM) ISS deployment in 2010

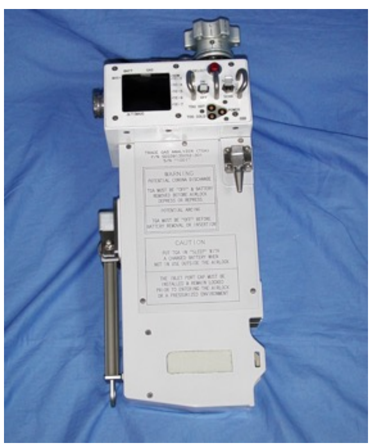
- Funded by NASA AEMC

Spacecraft Atmosphere Monitor (S.A.M.) ISS power on in August 2019

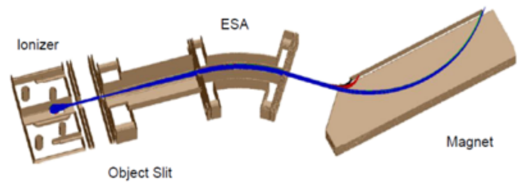
- Funded by NASA AEMC & AES

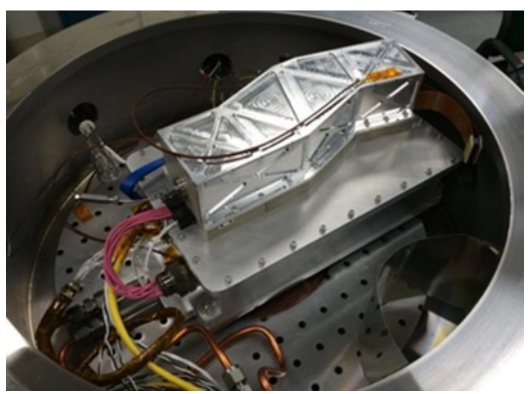
Past Mass Spectrometer Developments of the 389Team

Linear Quadrupole

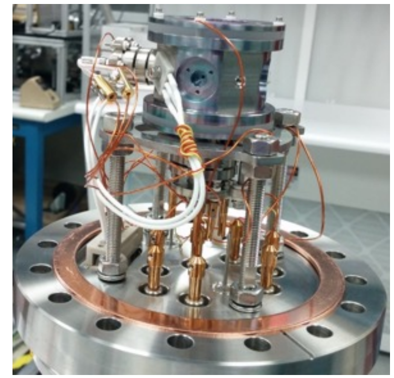


Magnetic Sector





Quadrupole Ion Trap



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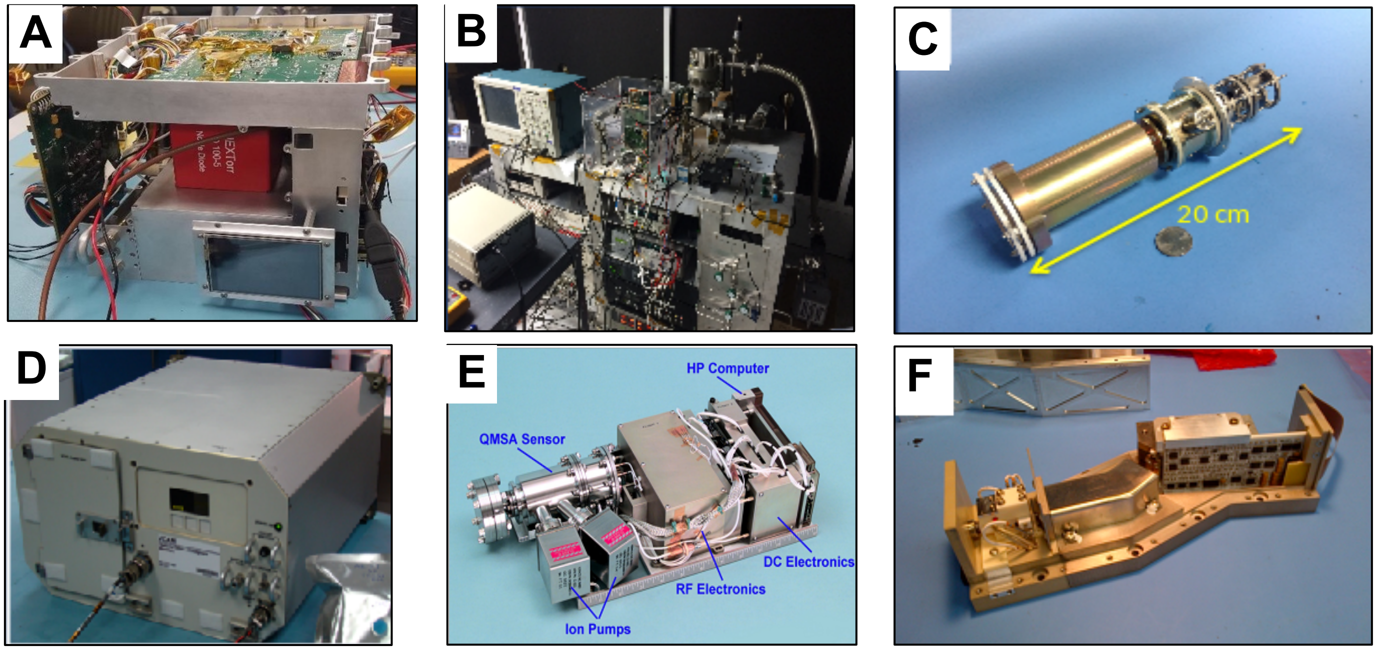
Rectilinear Ion Trap

Desired:

- Linear Ion Trap
- Triple Quadrupole MS
- TOF

Past Mass Spectrometer Developments of the 389Team

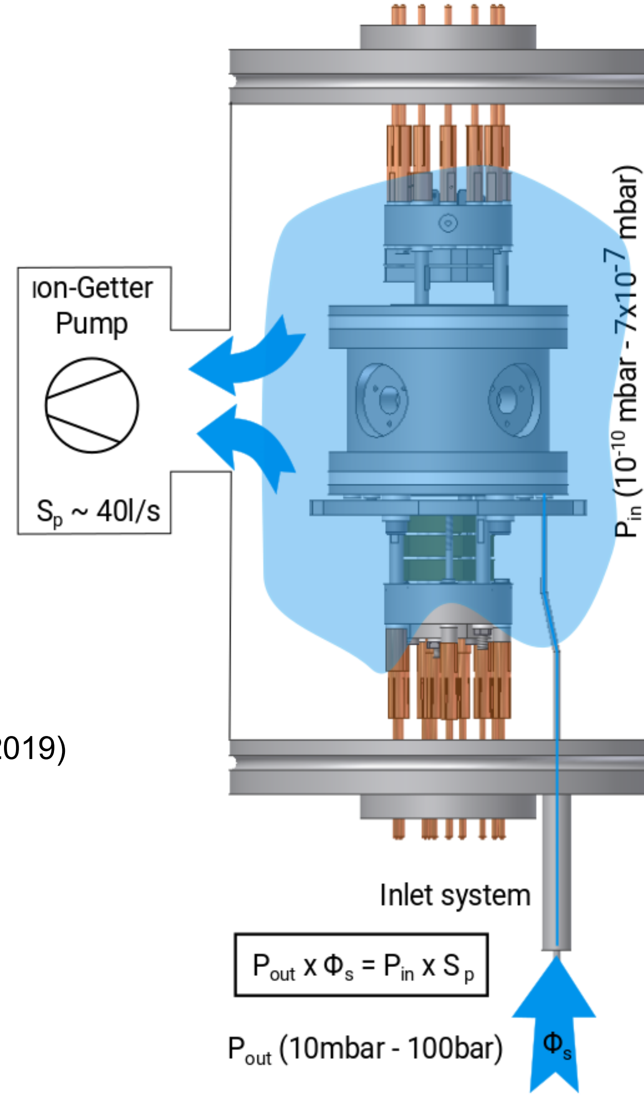


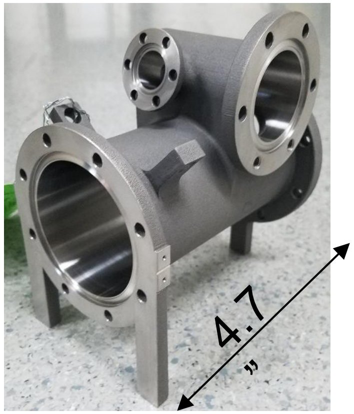
(A) Development Unit of Spacecraft Atmosphere Monitor (S.A.M)
(B) Geochronology and Atmospheric noble gas workstation.
(C) Flyby MS Sensor Head for Europa (MARINE) Prototype.
(D) VCAM deployed in the International Space Station's Destiny Laboratory. (Launched aboard STS-131 Discovery in 2010, operated for two years and came back on Dragon in 2013)
(E) The JPL Quadrupole MS Array - QMSA (2" in length - the smallest analytical linear quadrupole mass spectrometer sent to space, pictured here with electronics for the Trace Gas Analyzer - TGA).
(F) The JPL Miniature Mass Spectrometer - MMS, (a miniature magnetic sector MS - developed to be deployed on the Resource Prospector Mission - RPM to the South Polar Region of the moon)

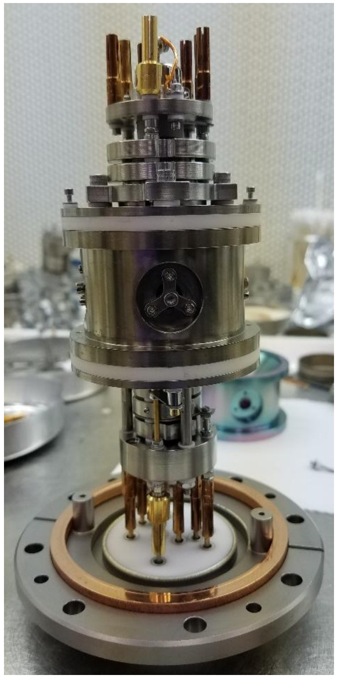
Components: Subsystem of QIT-MS

- QITMS* base pressure high 10^{-11} torr
- Operates without He buffer gas
- Different modes of operation (dynamic, static, resonant ejection)
- S.A.M** operating pressure ~$5x10^{-9}$ torr
- S.A.M. operating sensitivity $5x10^{12}$ cnts /torr/sec (dynamic)
- Inlet = fussed silica tube (single)
- Allows for MCA every 2 sec

*QITMS = Quadrupole Ion Trap Mass Spectrometer
**S.A.M. = Spacecraft Atmosphere Monitor (launch 2019)



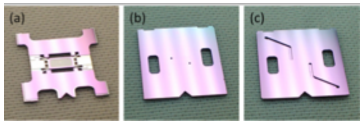




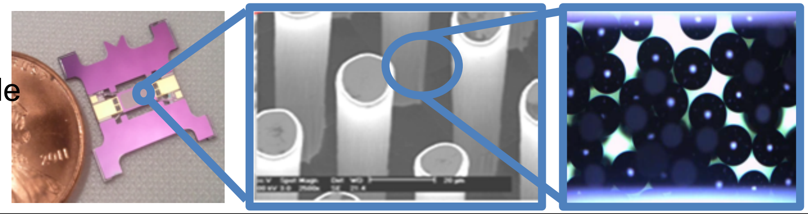
Component development: MEMS Gas Chromatography

Developed a variety of chip-based gas chromatography components that can be mixed and matched to give complete systems (or coupled to mass spectrometers) for a variety of planetary and human applications

Pre-Concentrator (PC)

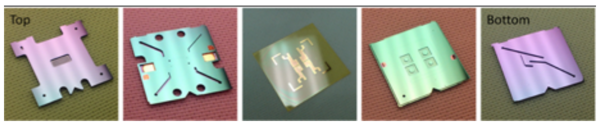


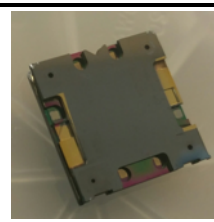
Heater/carboxen/inlet-outlet layers

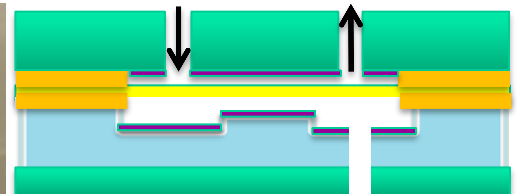


- Carboxen 1000
- ~200 µm particles
- ~10 Å pore diam.

Micro-Valve (MV)

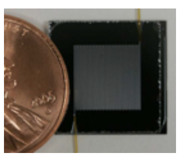


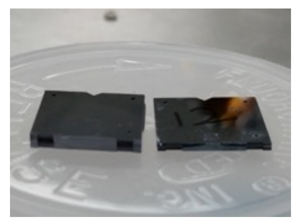




- Four microvalves are integrated in a chip: Sample, Vent, Carrier, and Injection.
- All the valves are electrostatic.

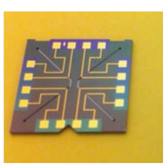
Gas Chromatograph (GC)

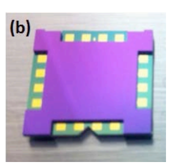




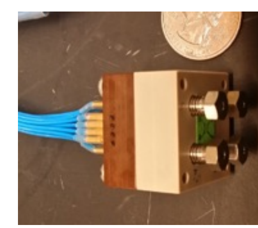
- 1 m length x 86 µm diameter chip dynamically coated.
- Serpentine column is superior to spiral design.
- A novel turn geometry to counteracts the dean vortices producing lower dispersion.
- Chips can be stacked to increase column length.

Thermal Conductivity Detector TCD)



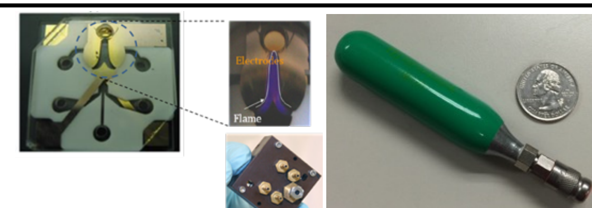


- Quantitative.
- Smallest detector package for gas chromatography.
- The TCD chip comprises two Si layers the footprint of which is only 14 x 14 x 0.5 mm^3.
- Minimum detection leve: 24.36 ng/ml (w/o pre-concentration).



Flame Ionization Detector (FID)

- Minimum detection level: 1 ng of hexane (w/o pre-concentration).
- Sensitivity: 84 mC/gC (at least four times higher than of any published micro-FID).
- Can be coupled to a MEMS electrolyzer or miniature metal-hydride H_2 tank.

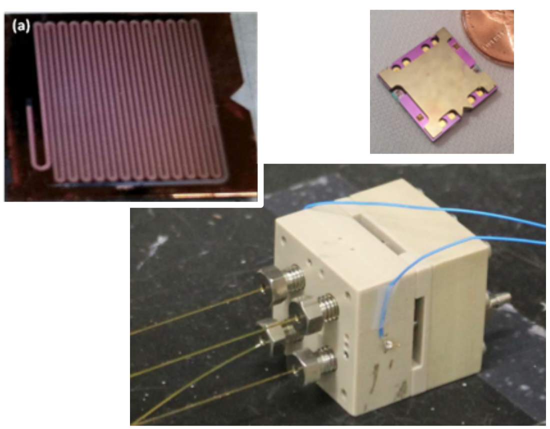


JPL/Caltech MEMS-based Chromatography

Gas Chromatography (GC)

- Can be coupled to a MS
- Very fast
- Can separate volatile small molecules
- Need to derivatize amino acids, fatty acids, etc.

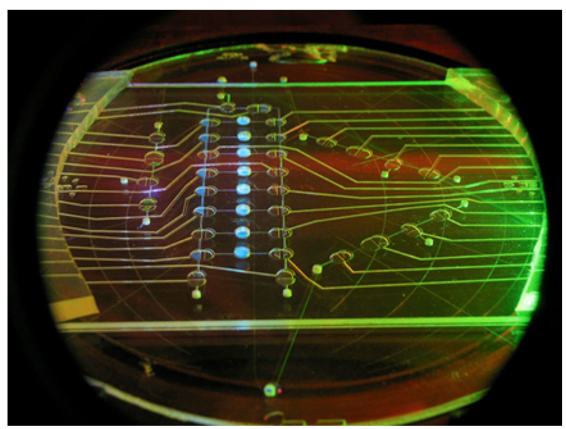
Madzunkov, S.M., MacAskill, J.A., Simcic, J., Kidd, R.D. & Darrach, M. (2013). Recent developments in gas chromatographs and mass spectrometers for crewed and robotic space missions. *J. Am. Inst. Aeronautics & Astronautics*. Electronic 2012-3453.



Capillary Electrophoresis (CE)

- Coupled to laser-based fluorescence detector
- Very sensitive/specific
- Can separate small molecules to macromolecules

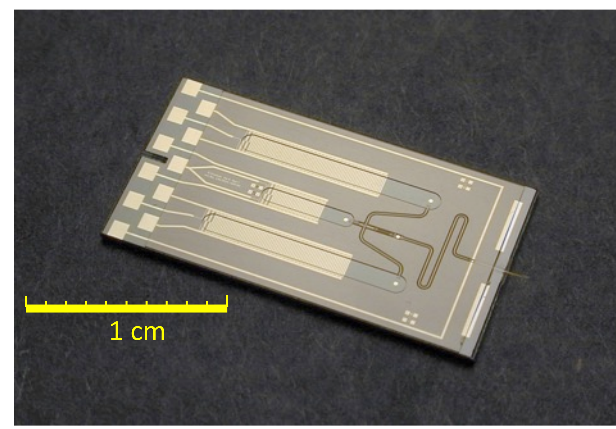
Willis, P. A., Stockton, A. M., Microchip Capillary Electrophoresis for In Situ Planetary Exploration. In *Capillary Electrophoresis and Microchip Capillary Electrophoresis*, John Wiley & Sons, Inc.: 2013; pp 277-291.



High Performance Liquid Chromatography (HPLC)

- Can be coupled to a MS
- Well suited for non-volatiles
- Can separate small molecules to macromolecules
- No derivatization required

Xie, J., Miao, Y., Shih, J., Tai, Y.-C. & Lee, T.D. (2005). Microfluidic platform for liquid chromatography-tandem mass spectrometry analyses of complex peptide mixtures. *Anal. Chem.* 77, 6947-6953.



Piezo-electric Valve for Atmospheric Descent Sampling

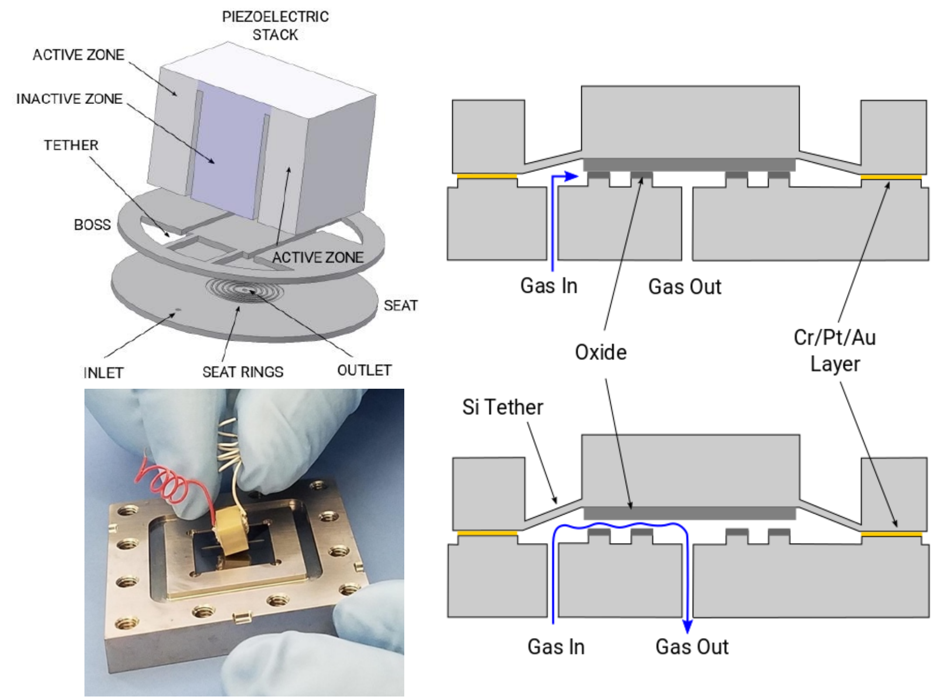
New Science Enabled:

- Gas compositions of Venus' atmosphere
- Gas composition of Saturn's atmosphere
- Noble gas ratios of Venus' and Saturn's atmospheres
- Trace gas molecules, ppb levels of Venus' and Saturn's atmospheres.
- Descent profile of all the species mentioned above, measured every 2 minutes.

Target Bodies: gas giants, planetary atmospheres, planetary body flyby, atmospheric probes

Key capabilities:

- Withstanding pressure difference of 100bar
- Capable of operating up to 150^{o}C
- No power consumption
- Response time on the order of ms
- Continuous regulation of gas flow
- Pulse or static mode
- Lightweight and durable



Schematic view of the piezo valve (top left), fabricated unit (bottom left), and principle of operation (right).

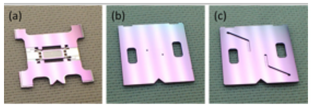
Path forward:

- Continue fabricating new valves
- Design lighter package
- Bond PZT straight to Si wafer

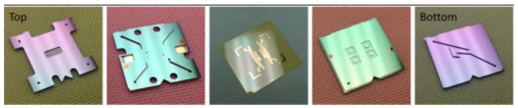
Co-Is: Choonsup Lee, Dragan Nikolic

S.A.M. Spacecraft Atmosphere Monitor

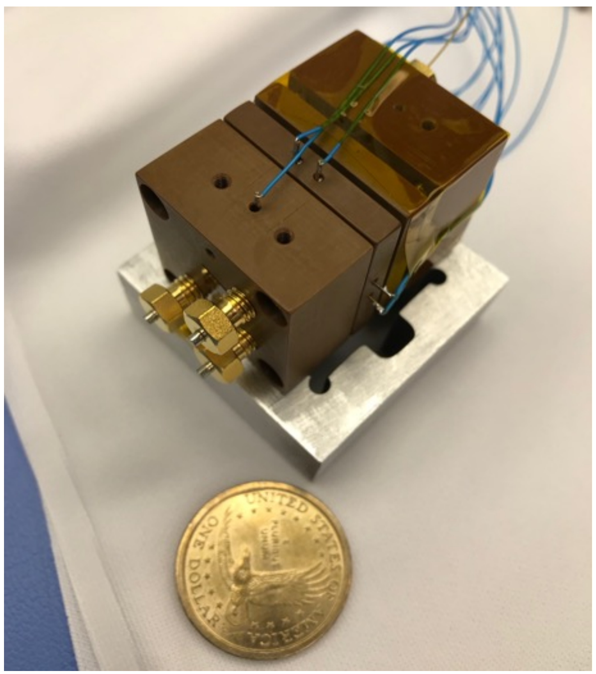
PC layer

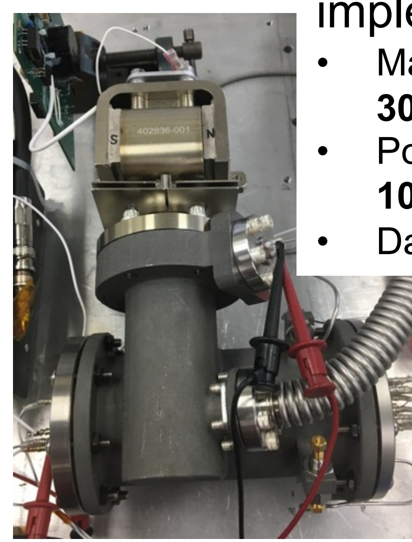


Valve layer



GC column



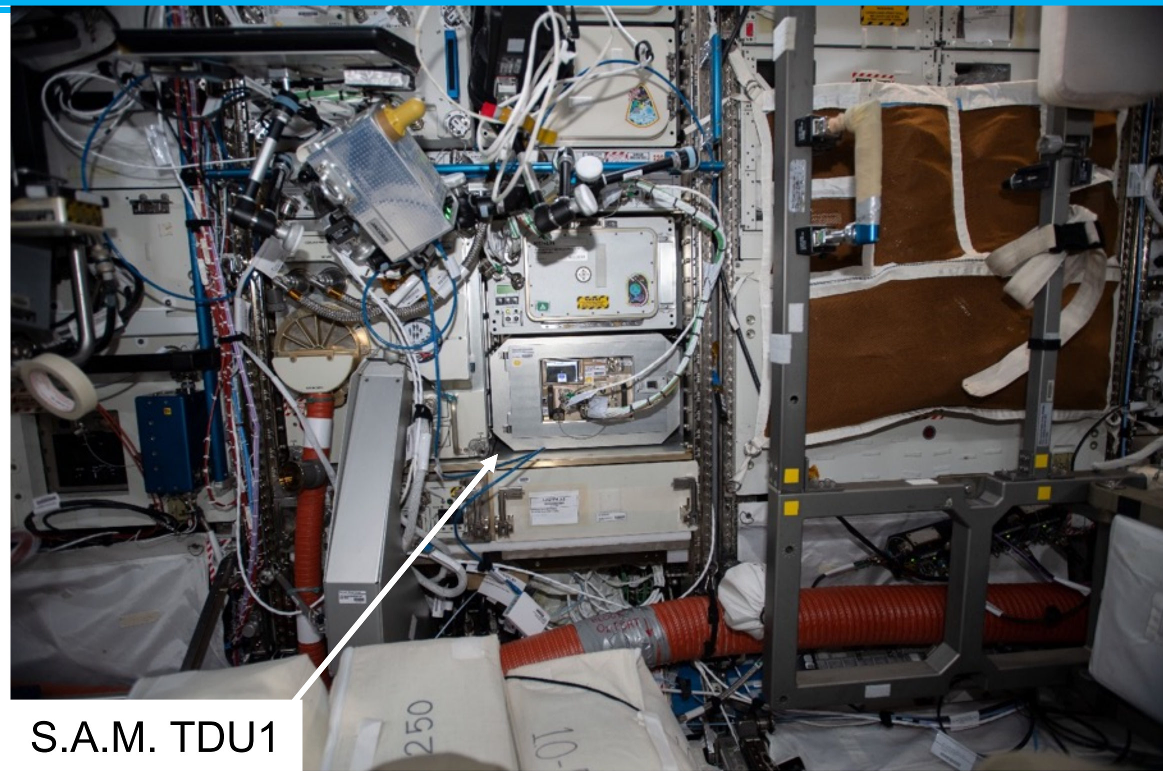


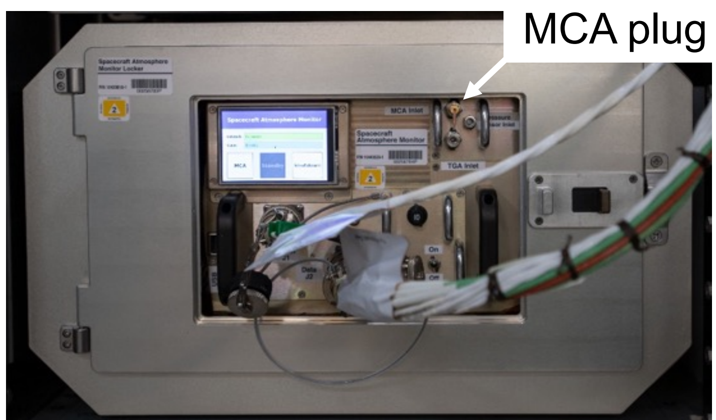
Flight implementation:

- Mass: (2011, VCAM) **30 kg,** (2019) **7 kg**
- Power (2011, VCAM) **100 W,** (2019) **30 W**
- Data rate is similar

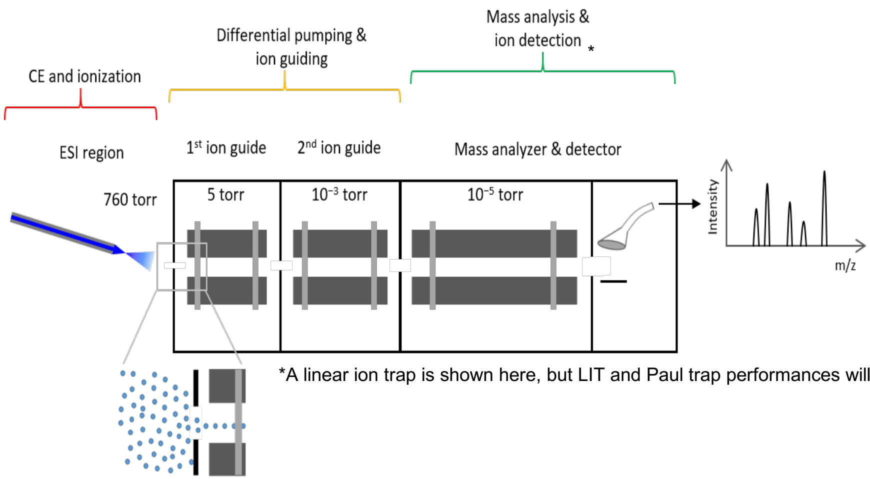
S.A.M. Spacecraft Atmosphere Monitor

- S.A.M. TDU1 installed & Powered On - Aug 8, 2019
- MCA plug removed Aug 9, 2019
- Nominal in-orbit checkout completed on Aug 9, 2019
- Detailed MCA performance analysis underway

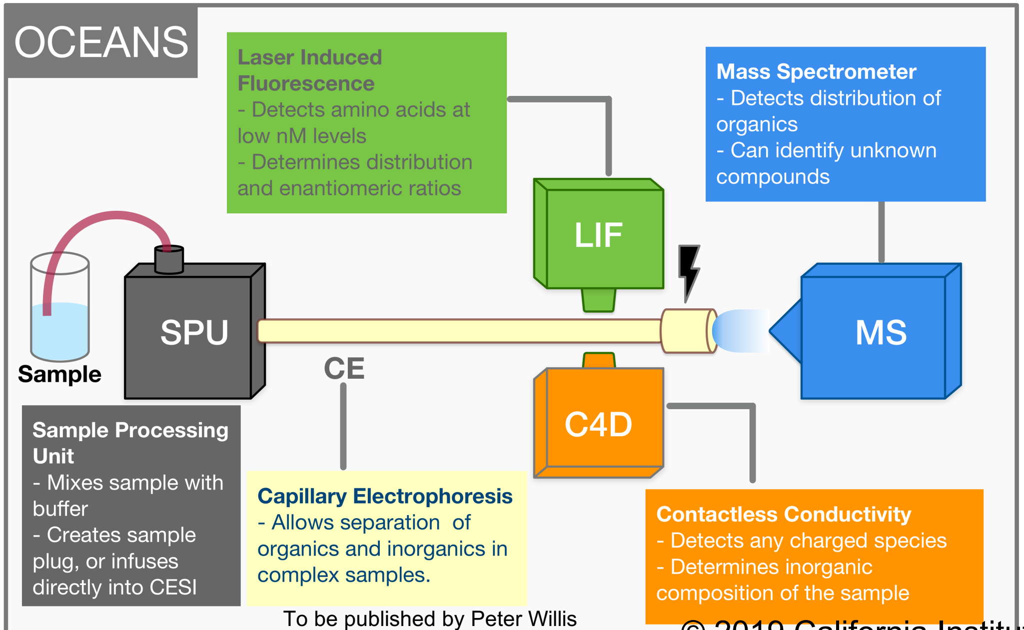




Ocean Worlds Life Surveyor –OCEANS CE-ESI-MS



*A linear ion trap is shown here, but LIT and Paul trap performances will be compared



The goal of OCEANS (Organic Capillary Electrophoresis Analysis System) is to design, build, and demonstrate an in situ chemical analyzer that can detect and characterize organic compounds.

The OCEAN Worlds Life Surveyor (OWLS) is funded under the JPL NEXT Program.

Goal to build and field test (Borup Bjord Pass in the Canadian High Arctic) prototypes in preparation to select instruments for possible missions to Enceladus, or Europa

Mass Spectrometer is part of Organic Capillary Electrophoresis Analysis System (OCEANS)

Electro**s**pray **I**onization coupled to Mass Spectrometry (ESI-QIT-MS) for broad-based detection and characterization of collections of organic molecules.

Capillary Electrophoresis (CE) will be coupled to ESI-QIT-MS. It allows to analyze organics at ppb levels, with 2% accuracy for relative amino acid abundances.

Life detection hinges upon identifying certain organic molecules

Amino acids are the building block of proteins and their distribution provide distinct biosignatures.

Water and Hydrate Isotopes via a Rapid Laser Sensor (WHIRLS)

Target: Comets, Primitive bodies, Mars evaporites (and ice), Icy moons, anywhere with water ice

Science:

- Understanding our solar system's volatile evolution (and especially the origin of water on Earth) by mapping its distribution of water H & 0 isotopes with low-cost missions

Objectives:

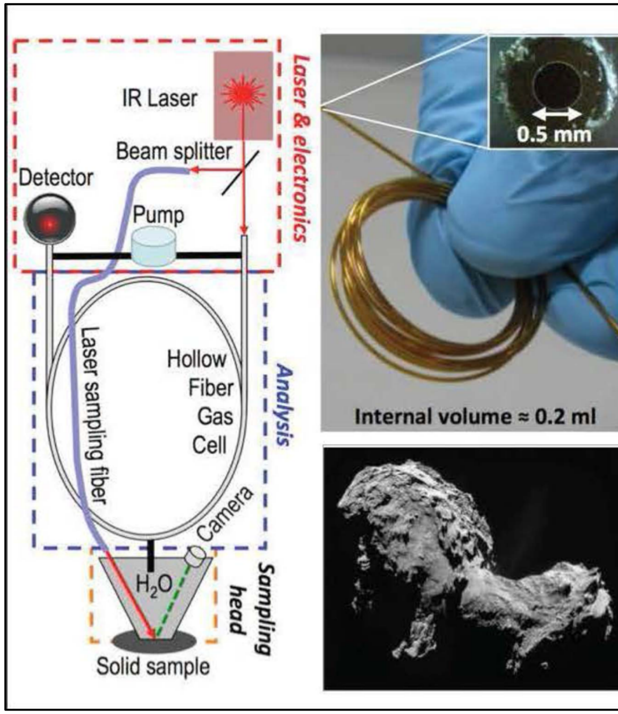
- Validation of a novel in situ instrument concept
  - Laser to release 5 nanomole water samples from ice and hydrated minerals
  - H & 0 isotope analyses by Capillary Absorption Spectrometry >10,000 times more sensitive than TLS and to ±1‰

To be achieved by these technical developments:

- Finalized design of the laser sampling system
- Finalized design of the sampling front end
- Produce the hydrophobic capillary
- Confirm or redefine where in the IR spectrum to measure ^{1}H, ^{2}H, ^{16}O, ^{17}O & ^{18}O
- Integrate the components & validate instrument
- Determine configuration & specs for a flight
- instrument's development.

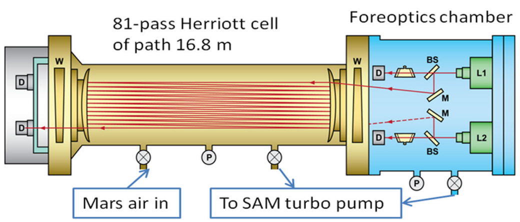
Cols:

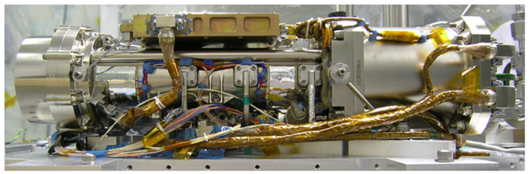
Lance Christensen, Ryan Briggs and Steve Vance - JPL
Jim Moran - DOE- Pacific Northwest National Lab.
Jason Kriesel and Jim Kelly - Opto-Knowledge Systems, Inc.



Schematic of the instrument (left). Laser heating releases water vapor into a 2m long hollow fiber (top right). The fiber is a wave guide giving optimum interaction between IR laser light and the vapor. It works like TLS to analyze H & O isotopes of water but also their small scale variations. Targets include safe landings on comets and primitive bodies (e.g. bottom right). We will prove the technology on H & O but in future want to work on other isotopes.

Tunable Laser Spectrometer (TLS) on Curiosity



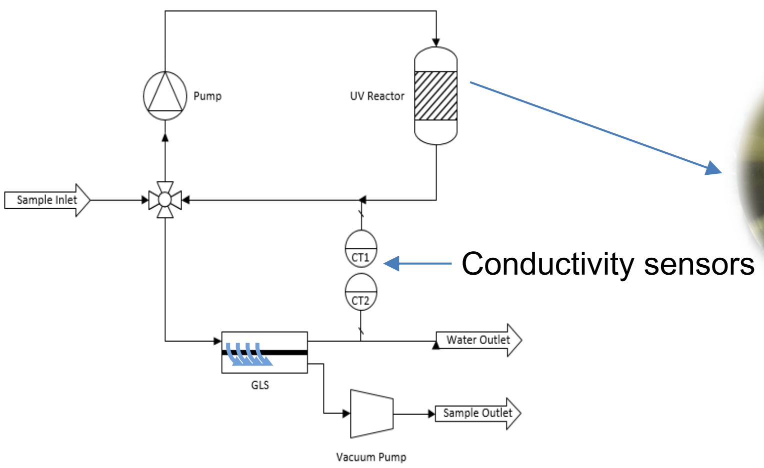


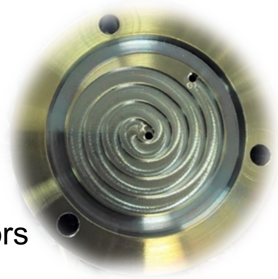
81-pass Heriott cell with path of 16.8m
fiber will have 2m

volume ~ 800 ml
fiber will have ≤ 0.2 ml

Miniature Total Organic Carbon Analysis (active R&TD miniTOCA)

Breadboard Development

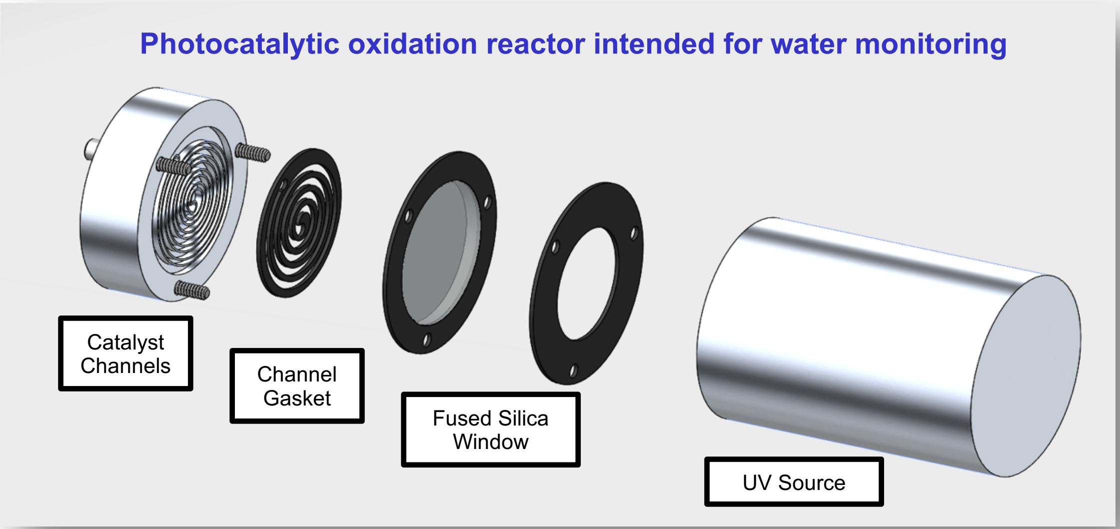




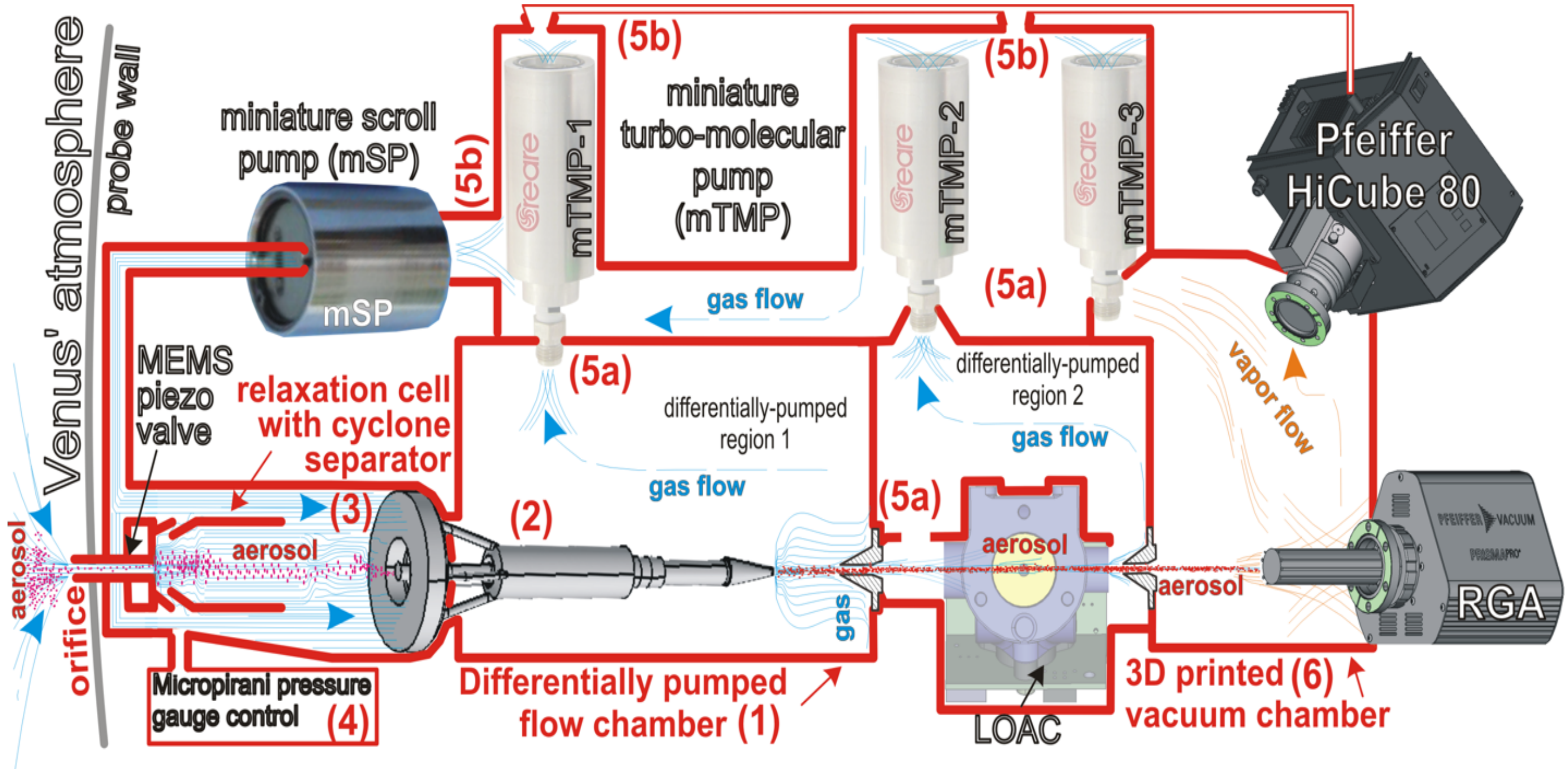
TiO_2 Photocatalytic surface

Optimization of components:

- **UV light source: initially 2W, now 6W**
- **Catalytic chamber:**
  - 3D Printed Laser Sintered Titanium
  - High surface roughness
  - Laser-cut gasket to seal channels
  - Heat-treated or coated using Atomic Layer Deposition (ALD) using TiCl4 and H2O (80nm) to excel oxidation
- **Initial results are promising. Further tests are ongoing.**
  - Goal is to get short and complete oxidation



Advanced NanoJet Aerosol Separator Apparatus

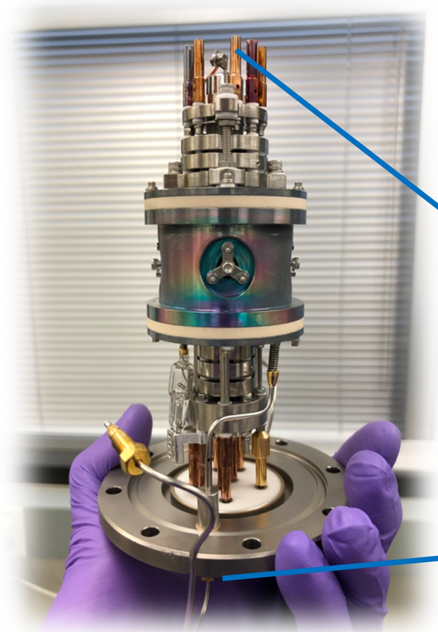


Under proposal phase:

- **Aerosol Separator (AS) as the gaseous sample inlet for any mass spectrometer operating in planetary atmosphere containing suspended aerosols, including liquid, icy, and metallic particles.**
- **High yield separation of heavier particles from the dominant gas phase at variable altitudes**
- **Tolerant to changes in atmospheric pressure of up to three orders of magnitude.**
- **Enables studies of chemical composition of aerosols at parts-per-billion sensitivity.**

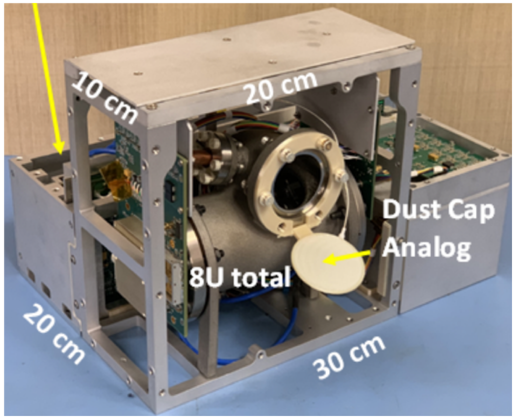
- **Primary target: UV absorber suspended in acidic aerosols in Venus' clouds**
- **Applicable also to: Aerial and surface missions to Titan and Mars and subsonic probe missions to the ice giants.**

Compact QIT-Mass Spectrometer for Lunar and Planetary Applications

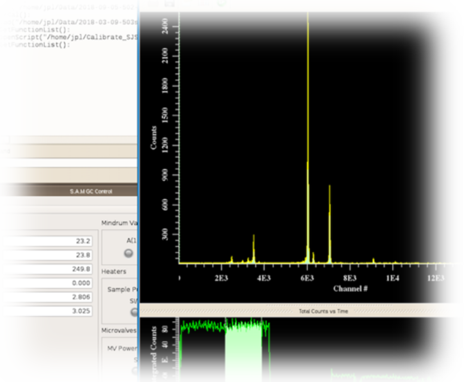


Sensor

J. Simcic, et al. *Miniature Gas Chromatograph Mass Spectrometer (GCMS) For Planetary Atmospheres In Situ Studies*, 3rd International Workshop on Instrumentation for Planetary Missions, 2016

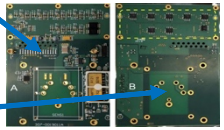


Prototype QIT-MS

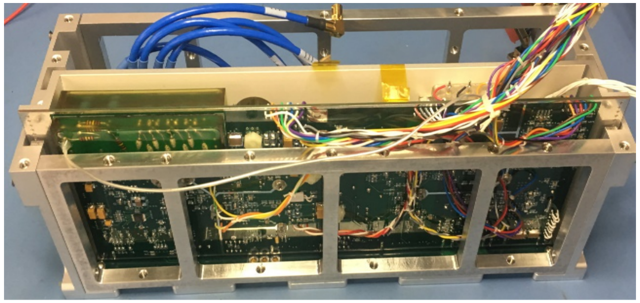


Integrated Software

D. Nikolić, et al., *Mass Spectra Deconvolution of Gaseous Mixtures Containing Volatile Organic Compounds*, 48th International Conference on Environmental Systems, article 313, 6 pages (2018).

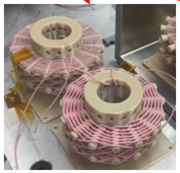


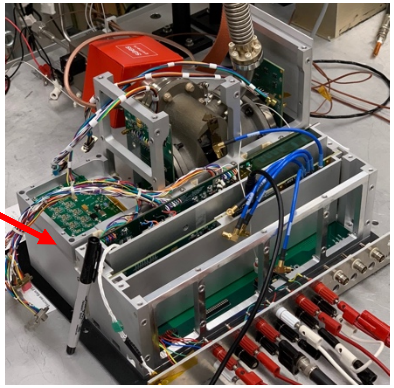
Cap electronics



Power and CPU Electronics

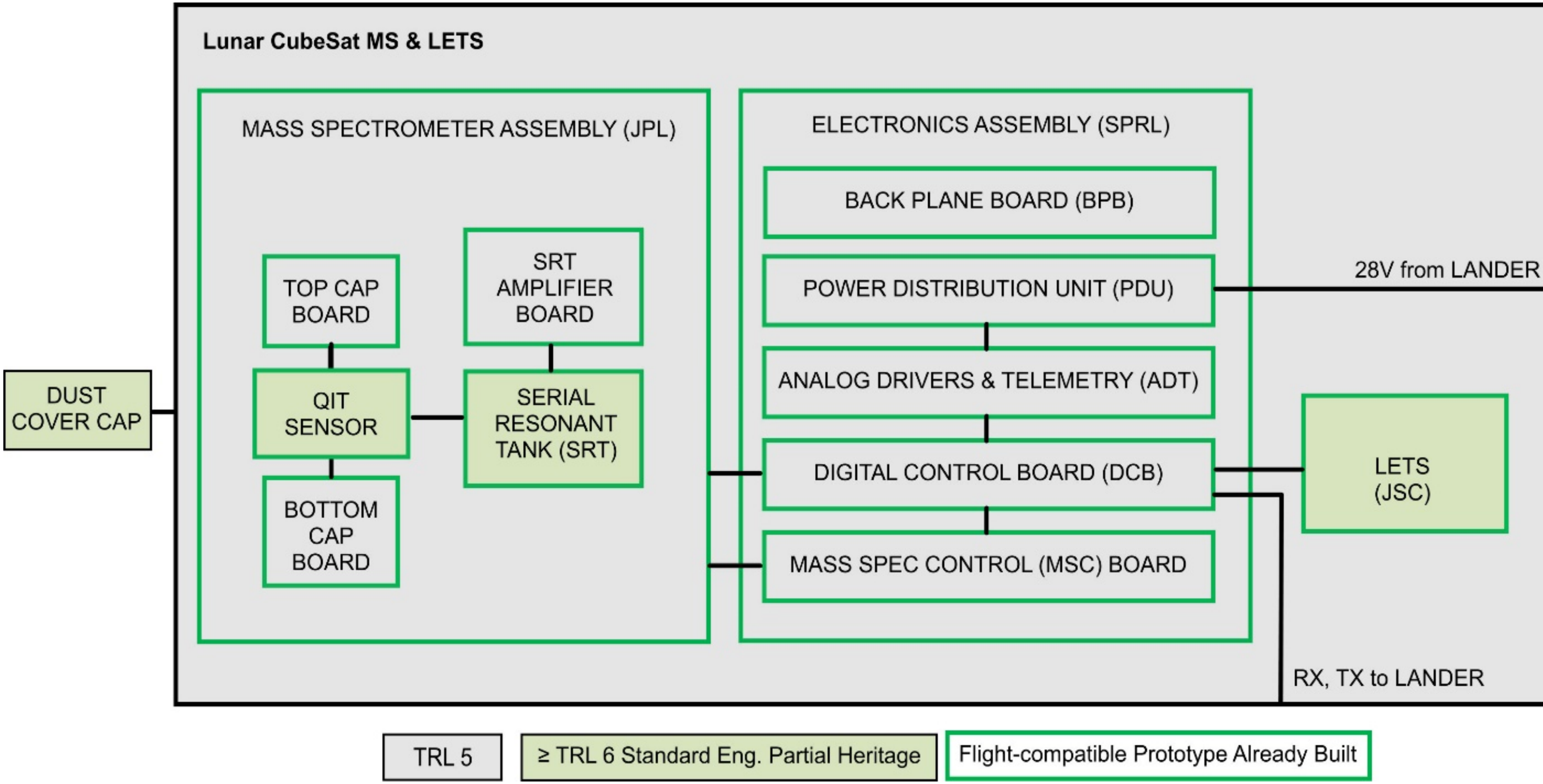
High Q diamond weave Litz wire coil





Mechanical Integration

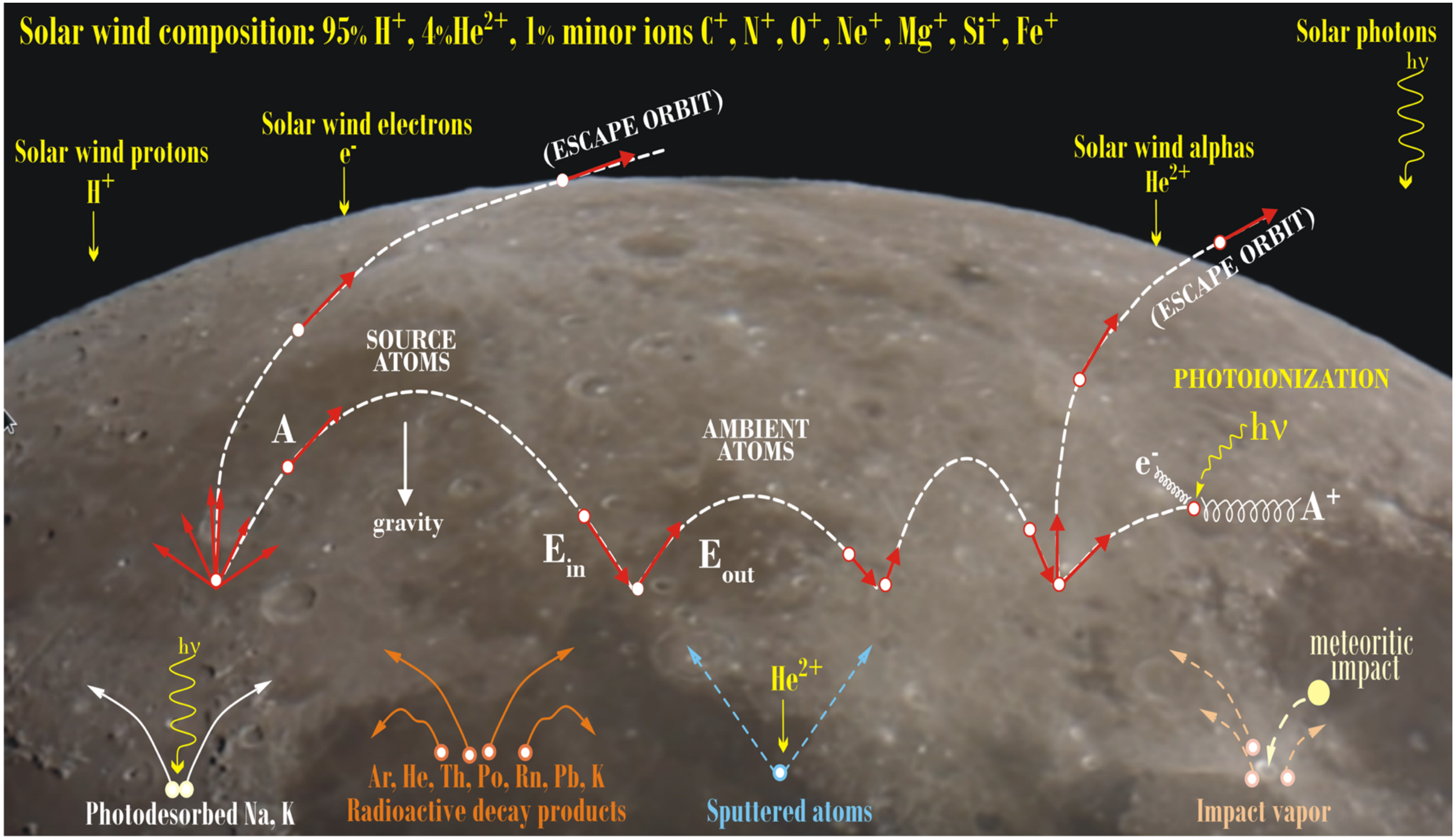
Readiness for Flight Implementation



Development over past years allowed to increase the TRL level of all components to 5 with design implementations to support TRL 6.

Lunar Exospheric Composition

- JPL QIT-MS with JSC Linear Energy Transfer Spectrometer (LETS) for **multi-day lunar surface exospheric and radiation investigations**.
- QIT-MS/LETS will be the first lunar instrument capable of **identifying and quantifying exosphere species with abundances ≥ 10 molecules/cm^3**



Publications

- D. Nikolic, D. Keicher, and F.-G. Fan, *Design of an Aerodynamic Lens for PM2.5 Chemical Composition Analysis*, 49th International Conference on Environmental Systems, 07-11 July 2019 Boston, Massachusetts, USA, ICES_2019_366 (2019).
- [16] D. Nikolic, J. Simcic, and S. Madzunkov, *Expected Performance of the QIT-MS Mass Spectrometer in Venus' Atmosphere*, 17th Meeting of the Venus Exploration and Analysis Group (VEXAG), November 6-8, 2019 in Boulder, Colorado USA, LPI Contribution No. 2193, id.8024 (2019).
- J. Simcic, J.C. Lee, S. Madzunkov, D. Nikolic, A. Belousov, *Piezo-Electric Inlet System for Atmospheric Descent Probe*, 16th International Planetary Probe Workshop & Short Course titled • Ice Giants: Exciting Targets for Solar System Entry Probes Exploration • 6–7 July 2019 Oxford University
- K.H. Baines, J.A. Cutts, D. Nikolic, S.M. Madzunkov, J.-B. Renard, O. Mousis, L.M. Barge, and S.S. Limaye, *An Aerosol Instrument Package for Analyzing Venusian Cloud Particles*, 17th Meeting of the Venus Exploration and Analysis Group (VEXAG), November 6-8, 2019 in Boulder, Colorado USA, LPI Contribution No. 2193, id.8010 (2019).
- [18] K.H. Baines, J.A. Cutts, D. Nikolic, S.M. Madzunkov, M.L. Delitsky, S.S. Limaye, K. McGouldrick, *The JPL Venus Aerosol Mass Spectrometer Concept*, 16th International Planetary Probe Workshop & Short Course titled • Ice Giants: Exciting Targets for Solar System Entry Probes Exploration • 6–7 July 2019 Oxford University
- S. M. Madzunkov, D. Nikolić, *Accurate Xe* Isotope *Measurement Using JPL Ion Trap*, J. Am. Soc. Mass Spectrom. **25**(11), 1841-1852 (2014).
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- Sotin, C & Avice, Guillaume & Baker, John & Freeman, Anthony & Madzunkov, Stojan & Stevenson, T & Arora, N & Dar-Rach, M & Lightsey, Glenn & Marty, Bernard. (2018). CUPID'S ARROW: A SMALL SATELLITE CONCEPT TO MEASURE NOBLE GASES IN VENUS' ATMOSPHERE. Conference: 49th Lunar and Planetary Science Conference (2018), At Houston, TX (USA)
- Murray, Vanessa & Pilinski, Marcin & Smoll, Eric & Qian, Min & Minton, Timothy & Madzunkov, Stojan & Darrach, Murray. (2017). Gas-Surface Scattering Dynamics Applied to Concentration of Gases for Mass Spectrometry in Tenuous Atmospheres. The Journal of Physical Chemistry C. 121. 10.1021/acs.jpcc.7b00456.
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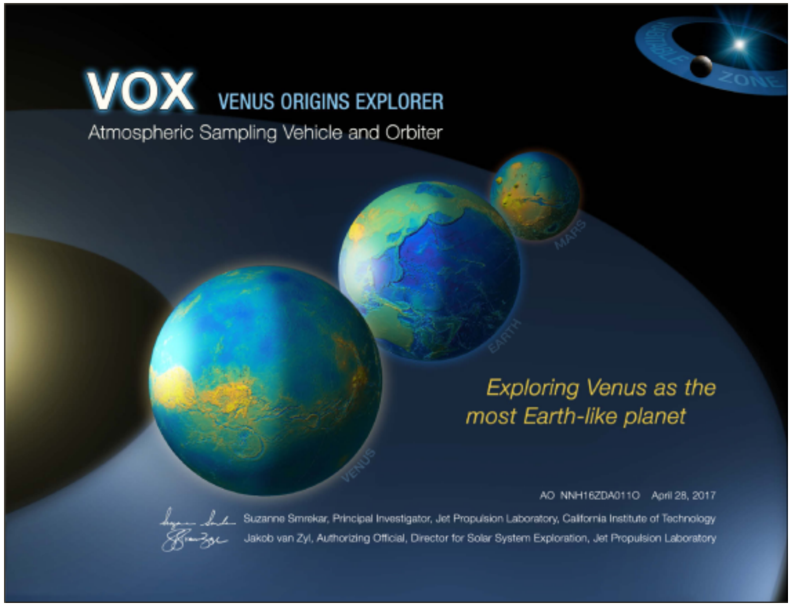
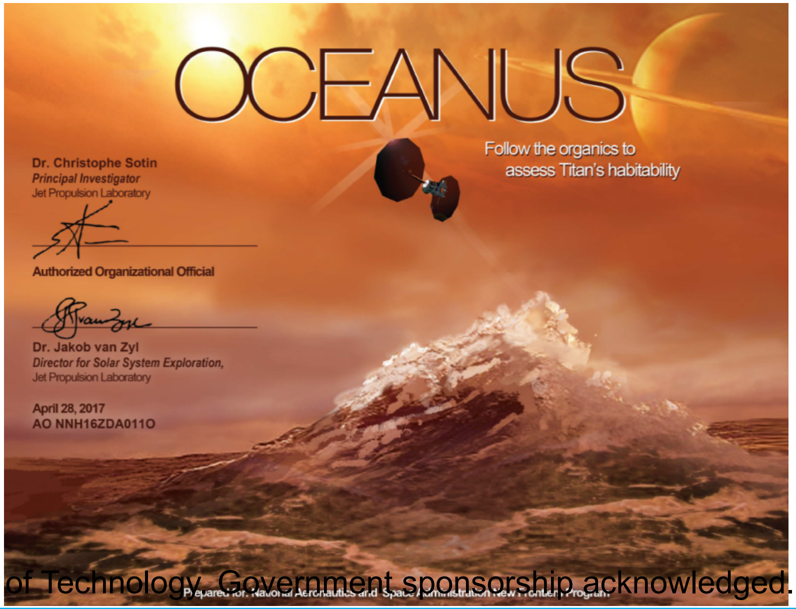
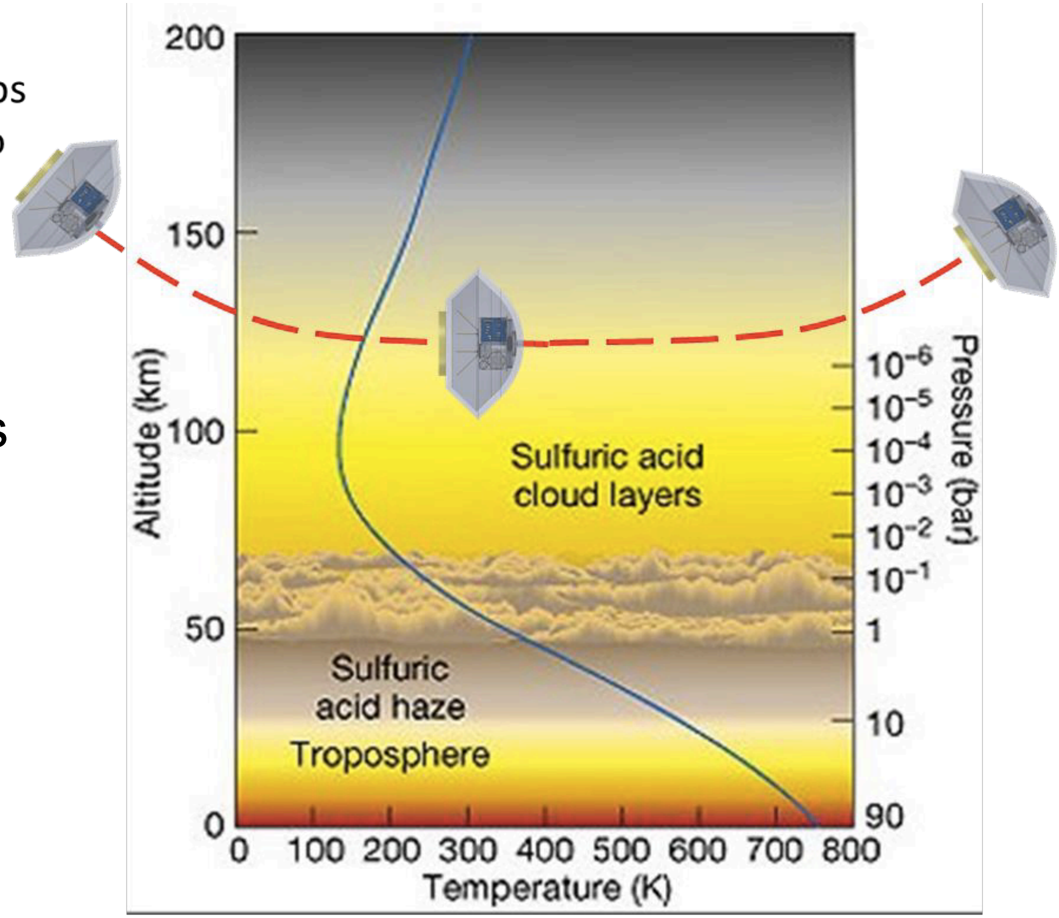
Past Mission Proposal Concepts





CUPID'S ARROW

Probe dips down to 120km



Atmospheric Entry Conditions

Entry velocity of 10 km/s
Target altitude of 110 km

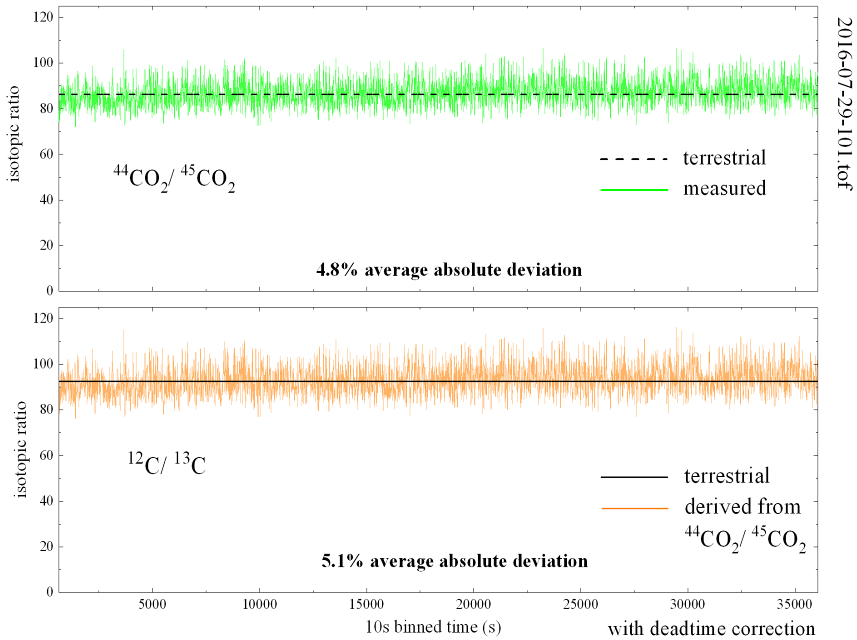
Homopause is between 119 km (evening terminator) and 135 km (night side close to the morning terminator) with a weak dependence on latitude (Limaye et al., 2017)

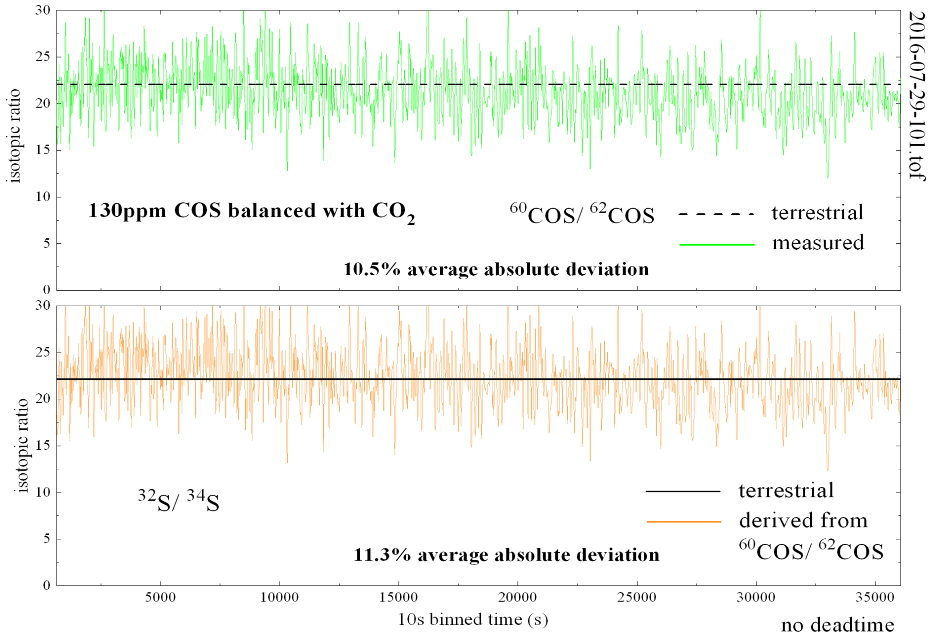
Pre-Decisional Information – For Planning and Discussion Purposes Only

Science Motivation

New Frontiers AO Science Objectives		Constituent	Required Accuracy	Projected JPL MS Performance
Physics and Chemistry of the Atmosphere, Thermochemical, Photochemical, and Dynamical Processes	Noble Gas Isotopes (Venus and Saturn)	**Concentration of major isotopes** (^{4}He, ^{20}Ne, ^{36}Ar, ^{40}Ar, ^{84}Kr, ^{130}Xe)	<10%	<3%
		Helium isotopes ($^{3}He/^{4}He$)	<5%	<3%
		Other major ratios e.g. ($^{20}Ne/^{22}Ne$, $^{36}Ar/^{38}Ar$, $^{82,83,86}Kr/^{84}Kr$, $^{129,136}Xe/^{130}Xe$)	<5%	<3%
		Minor isotopic ratios ($^{124\text{-}128}Xe/^{130}Xe$, $^{78,80}Kr/^{84}Kr$)	<25%	<5%
	Light Stable Isotopes	Venus: $^{14}N/^{15}N$	<5%	<3%
		Saturn: $^{13}C/^{12}C$ (methane)	<10%	<3%
		Saturn: D/H (hydrogen) and $^{14}N/^{15}N$	<10%	<3%
	Trace Gas Abundances	Venus: SO_2, OCS, H_2S, S_8	1 ppm at 10%	1 ppb at 10%
		Saturn: CH_4	<5%	<1%
		Saturn: H_2S	1 ppm at 10%	10 ppb at 10%
		Saturn: PH_3, P_2H_4, C_2H_6, C_3H_8	<10 ppm at 10%	<10 ppb at 10%

Findings – Measurements (isotope ratios, deadtime correction, rejection)





12C/13C Isotopes:

Measuring of 12C/13C isotopes from CO2. For accumulation of signal for 10s we obtained the 5% accuracy. The black solid and dashed and solid lines are indicating the true ratio values

32S/34S Isotopes:

Measuring of 32S/34S isotopes from COS. For accumulation of signal for 10s we obtained the 11% accuracy. The black solid and dashed and solid lines are indicating the true ratio values

Expected Performance based on Laboratory

Driving Measurement Requirement	Lunar Surface Observable	Instrument Performance Requirement		Projected Performance	Margin*
Determine which volatile species are present at the lunar surface at abundances ≥10 cm^{-3}	H, H_2, ^3He, ^4He, Ne, N_2, O_2, Ar, CH_4, CO, CO_2, Kr, Xe, OH, H_2O	Mass Range (Da)	1-140	0.75-230	65%
		Mass Resolution (m/Δm FWHM)	200	1000	400%
		Sensitivity (molecules/cm^3/sec)	0.001	0.0005	100%
		Target species partial pressure (Torr), 2:1 SNR	$\leq 1 \times 10^{-14}$	$\leq 1.3 \times 10^{-15}$	700%

Sources used in compiling the required LUNAR targets are:

1) 2013-2022 Planetary Decadal Survey, Visions & Voyages, p. 118, critical science goal for the moon and other inner solar system bodies: "Understand the Composition and Distribution of Volatile Chemical Compounds…"
https://www.nap.edu/login.php?record_id=13117&page=https%3A%2F%2Fwww.nap.edu%2Fdownload%2F13117

2) 2007 NRC Report: Scientific Context for Exploration of the Moon
https://www.nap.edu/login.php?record_id=11954&page=https%3A%2F%2Fwww.nap.edu%2Fdownload%2F11954
8a. Determine the global density, composition, and time variability of the fragile lunar atmosphere before it is perturbed by further human activity.
8c. Use the time-variable release rate of atmospheric species such as 40Ar and radon to learn more about the inner workings of the lunar interior.
8d. How water vapor and other volatiles are released from the lunar surface and migrate to the poles where they are adsorbed in polar cold trap.

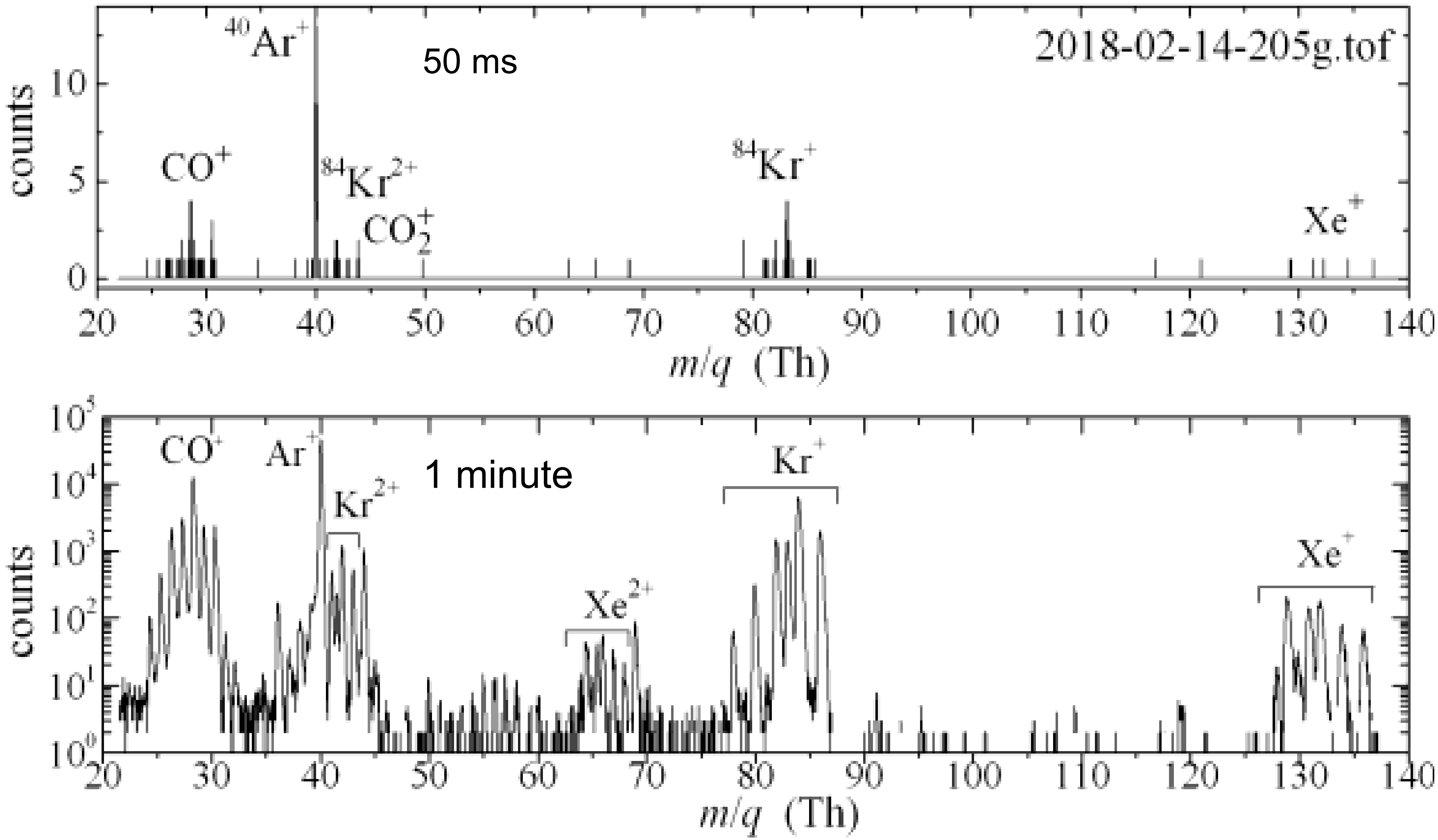
3) LEAG Specific Action Team Report, Goal 8a: "Systematically detect trace volatile species, like water, OH, and hydrocarbon in the exosphere."

4) LEAG Specific Action Team Report, Goal 8b: "Detect volatile transport from mid- to high-latitudes as a function of driving space environmental (solar storm, meteor stream) conditions."
https://www.lpi.usra.edu/leag/reports/vsat_report_123114x.pdf

5) HEOMD / Lunar Human Exploration Strategic Knowledge Gap (SKG) Special Action Team Report, September 2016: I-C, Regolith Volatiles, in situ. "Quality/ quantity/ distribution/ form of H species and other volatiles in nonpolar mare/highlands regolith."
https://www.nasa.gov/sites/default/files/atoms/files/leag-gap-review-sat-2016.pdf

Noble Gas Mass Spectrums

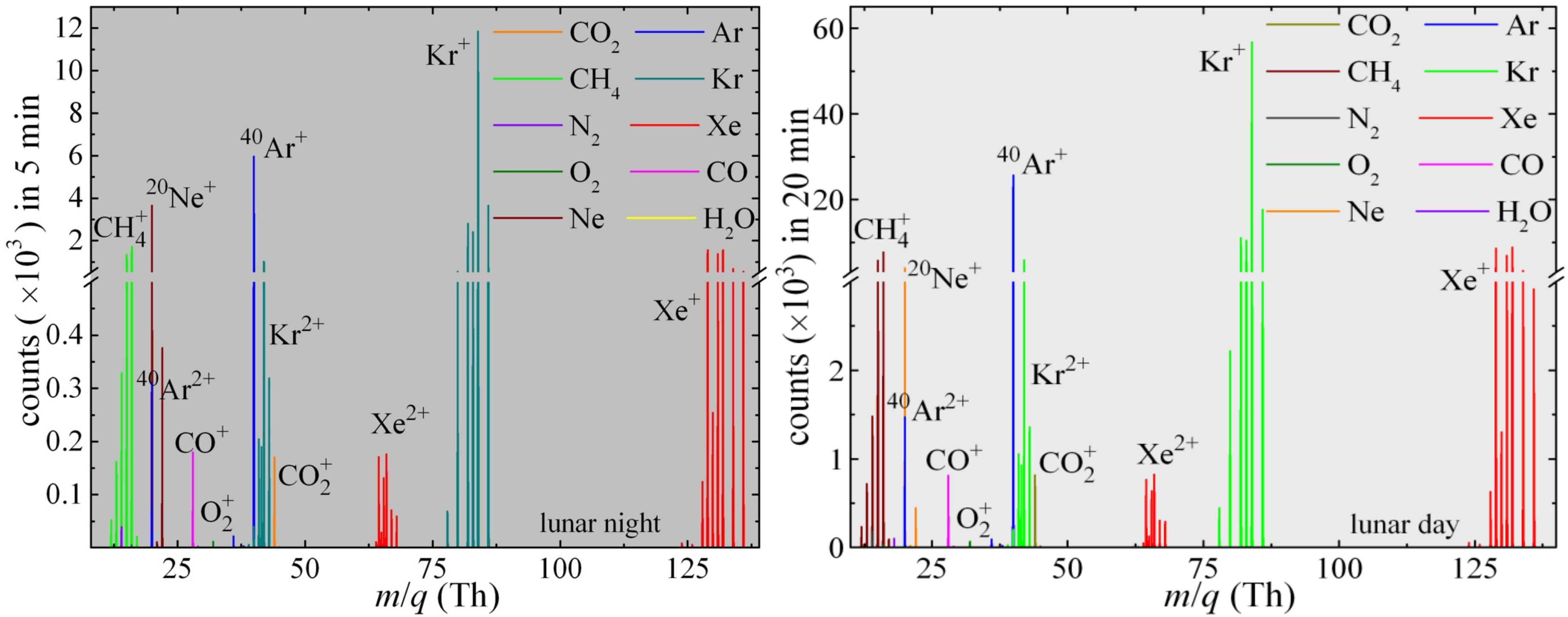
Isotope spectra of an aliquot of calibrating gas (1.7E-10 Torr of Kr and 1.3E-11 Torr of Xe) measured continuously **for 7 hours yielded a 0.6 ‰ precision on the 86Kr/84Kr ratio**



*G. Avice, A. Belousov, K. A. Farley, S. M. Madzunkov, J. Simcic, D. Nikolic, M. R. Darrach and C. Sotin, "High-precision measurements of krypton and xenon isotopes with a new static-mode quadrupole ion trap mass spectrometer," JAAS, Vol 34, January 2019

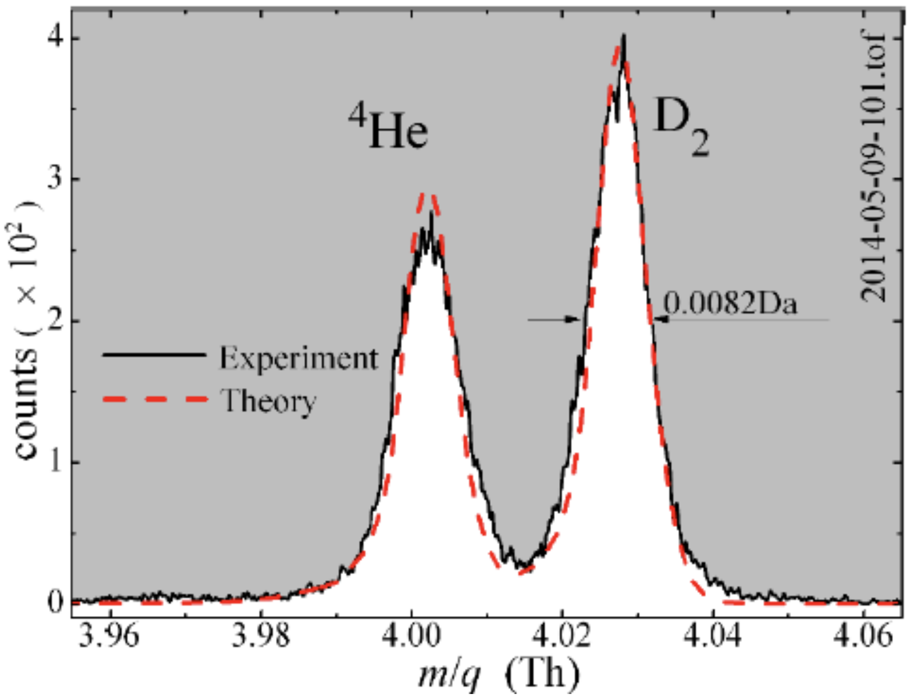
Predicted QIT-MS Response at Lunar Surface (diurnal)

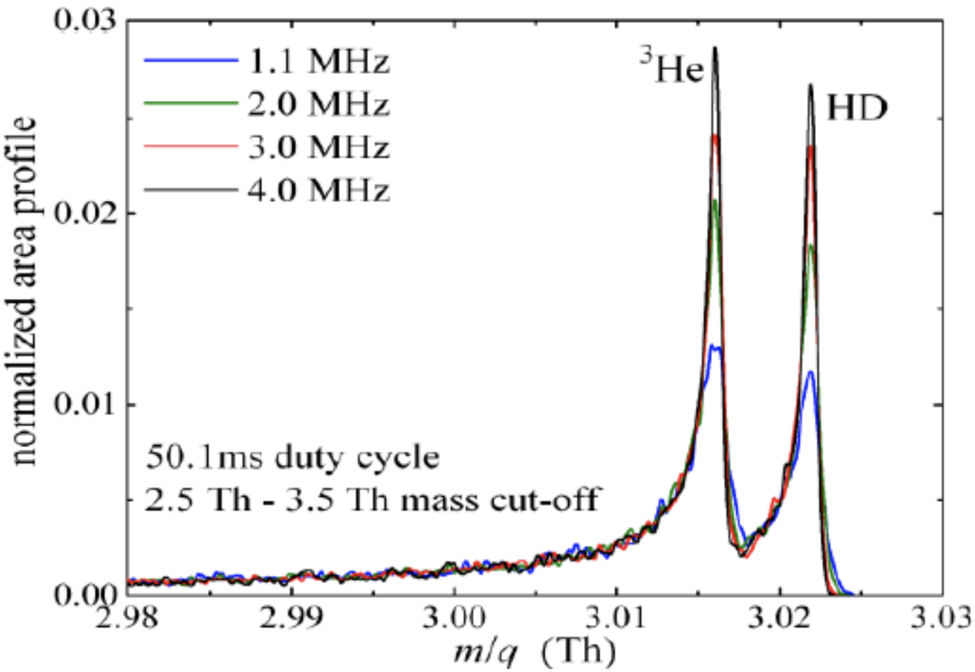
Simulation results with JPL lunar model (based on previously published in peer reviewed journals)



Measured High Resolution Mode

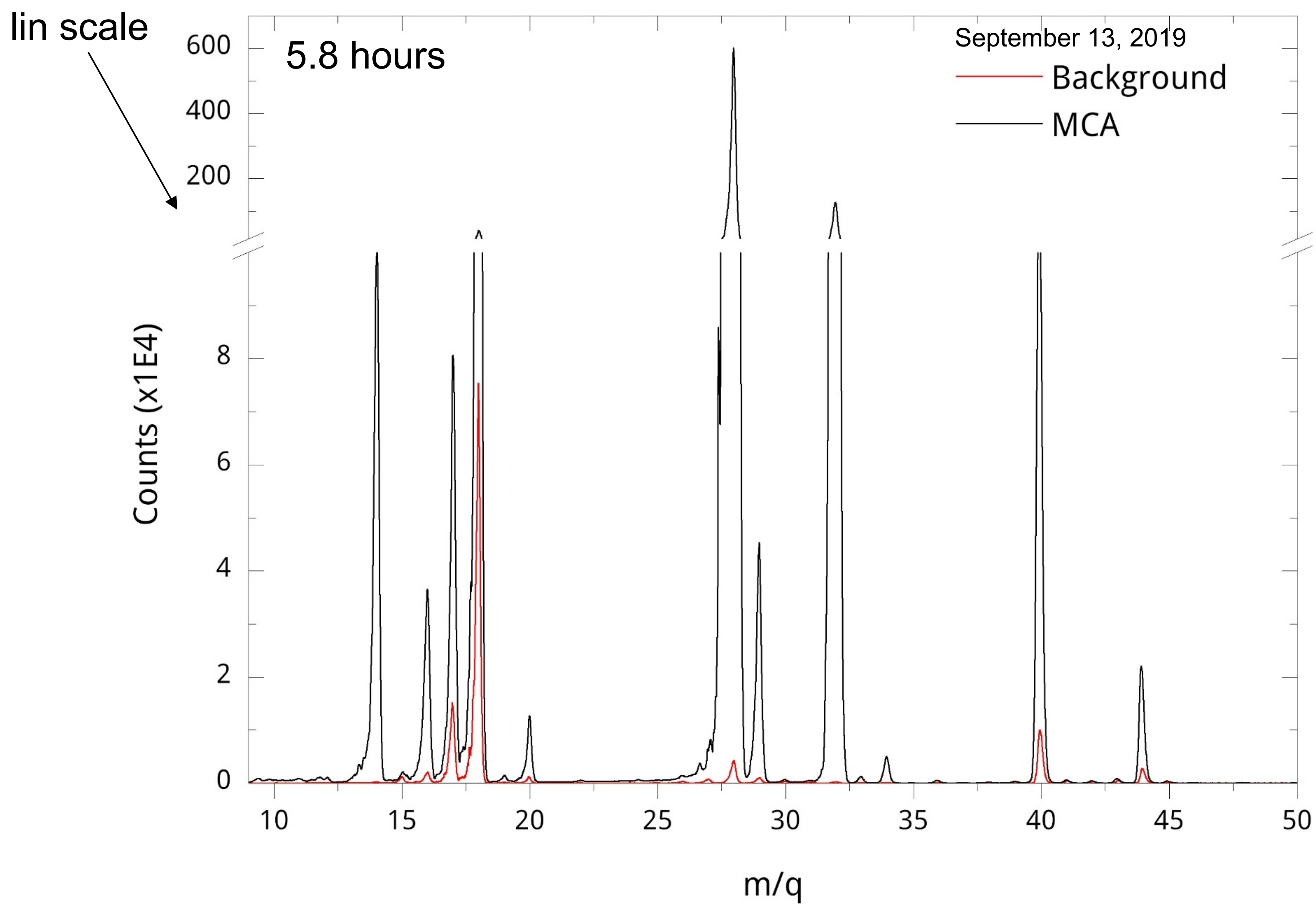
Measured and Modeled QITMS Mass Spectra. (Left) Measured QITMS spectra for 4He and D2 (dotted line) with a modeled 4He and D2 spectra. (Right) Modeled spectra for 3He and HD, at identical abundances, for various rf frequencies. The equal 3He and HD abundances are based on the published isotopic ratios in the lunar regolith [Wiens (2003)] and the expected AtLAS H2 instrument off-gassing after < 1 day of lunar surface bakeout of.



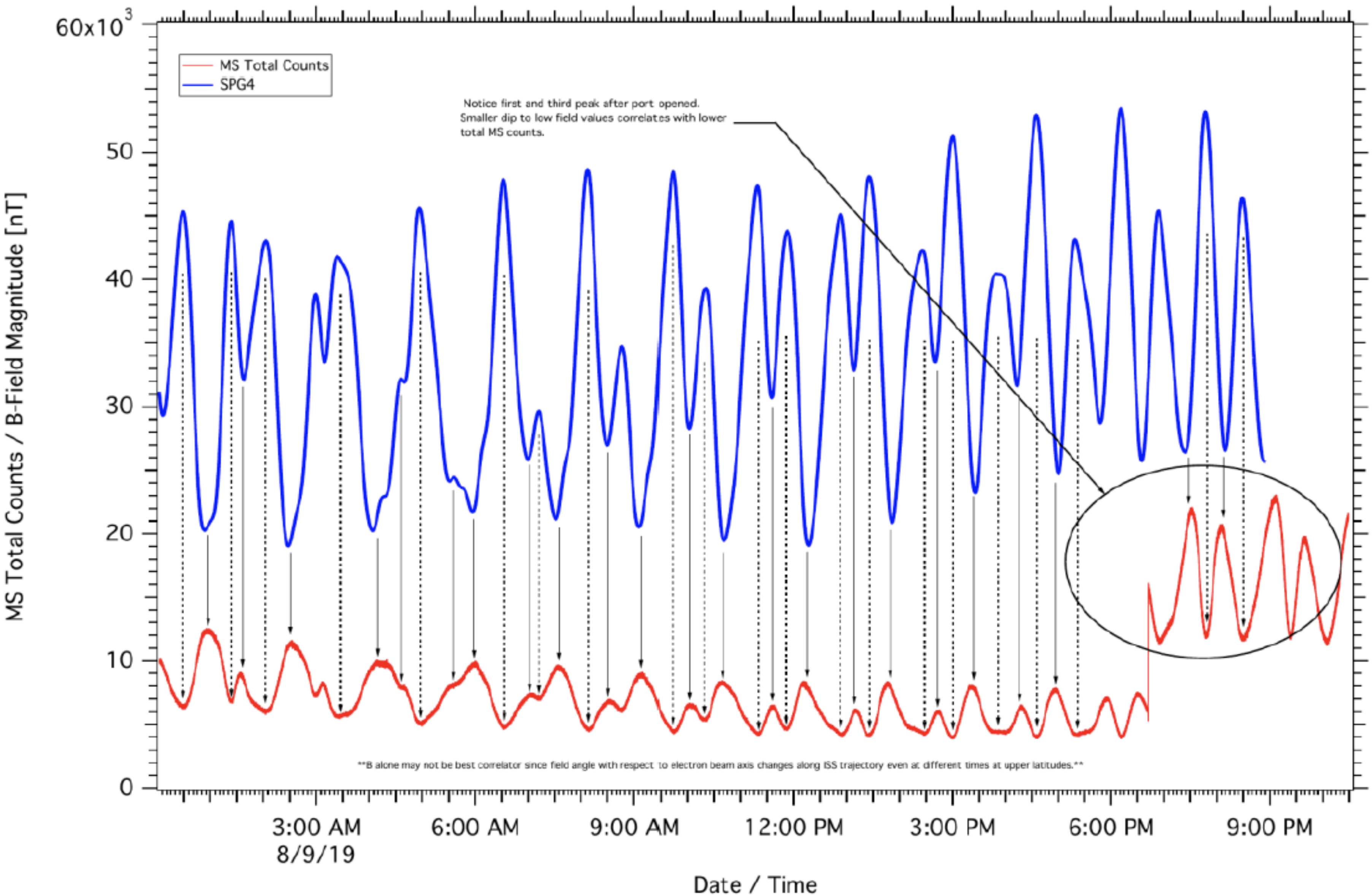


Nikolic, D., Madzunkov, S.M., Darrach, M.R., “Computer Modeling of an Ion Trap Mass Analyzer, Part I: Low Pressure Regime”, J. Am. Soc. Mass Spec., 26, 2115-2124 (2015)

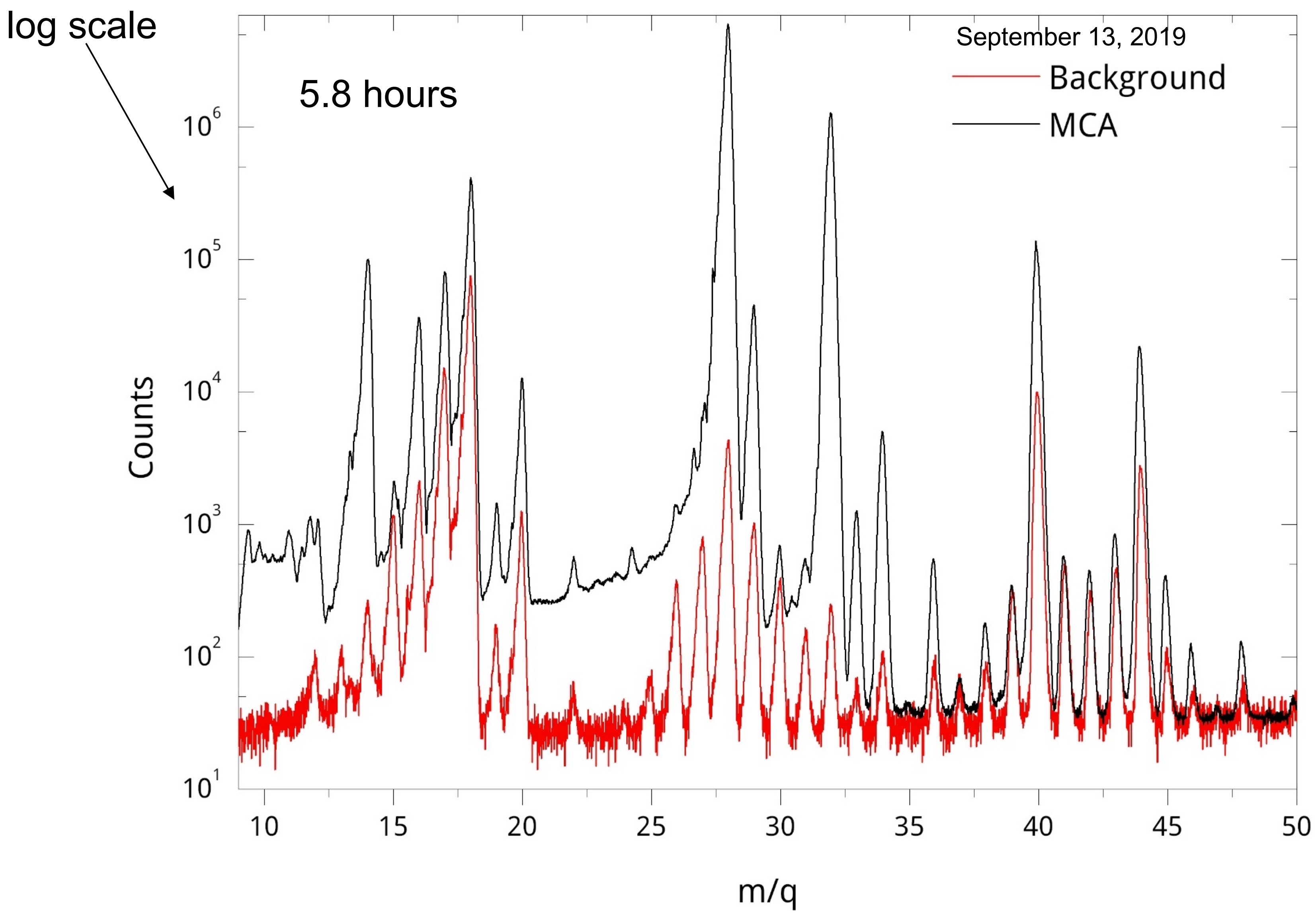
S.A.M. MCA with underlying background



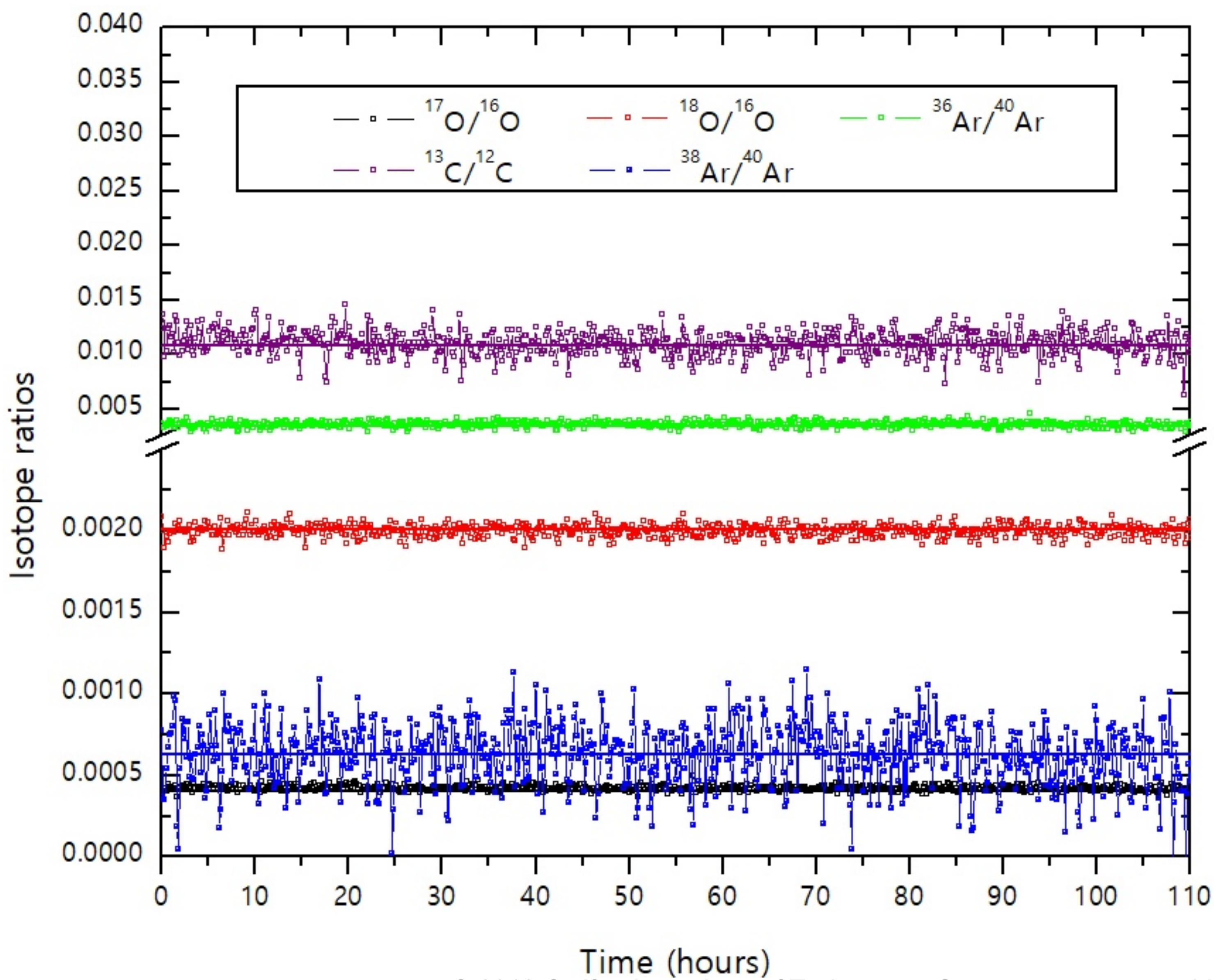
S.A.M.: Variation of total counts due to geomagnetic field



S.A.M. MCA with underlying background



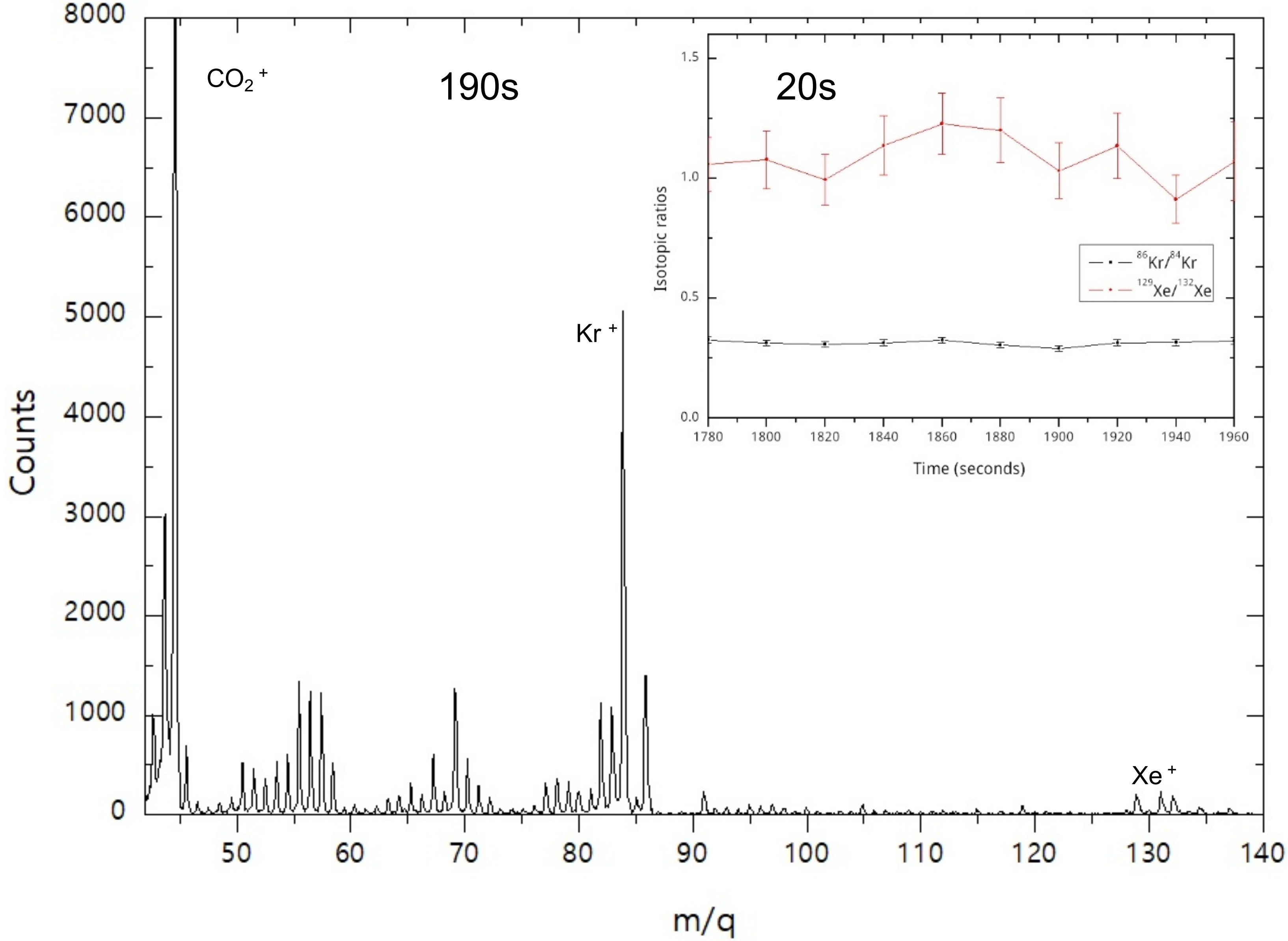
Isotopic long term stability from S.A.M. data (calibrated)



Isotopic ratio long term stability from S.A.M. data

Meas. duration		1 hour	10 hours	65 hours
$^{17}O/^{16}O$	Mean	0.000421(7)	0.000426(2)	0.0004250(9)
	SEM	1.7%	0.5%	0.2%
$^{18}O/^{16}O$	Mean	0.00197(3)	0.002000(6)	0.002000(2)
	SEM	1.3%	0.3%	0.1%
$^{36}Ar/^{40}Ar$	Mean	0.00359(9)	0.00354(4)	0.00361(2)
	SEM	2.5%	1.1%	0.4%
$^{38}Ar/^{40}Ar$	Mean	0.00058(8)	0.00063(3)	0.00064(1)
	SEM	13.1%	4.0%	1.4%
$^{13}C/^{12}C$	Mean	0.0119(6)	0.0115(2)	0.01105(6)
	SEM %	5.2%	1.2%	0.5%

Isotopic Measurements of Laboratory Air



Conclusions

- Future QIT-MS which have a compact form factor (8U, < 10kg) and low power consumption (<30W)
- Accuracy / Precision match with laboratory size magnetic sector MS at shorter integration times
- Proposing for near-future flight opportunities to raise the TRL level
  - Discovery and New Frontiers
  - Instrument developments
  - Internal funding

Future Roadmap

- ISS and future Moon/Mars mission crew safety
  - Air
    - Composition
    - Combustion
  - Water quality
  - Volatiles detector
    - In habitats
    - From soil
- Science mission to
  - Moon
  - Comets
  - Venus
  - Titan and Ice Giants
  - Others
- Seeking out for collaboration and PostDocs

S.A.M. is in the ISS but what is next?

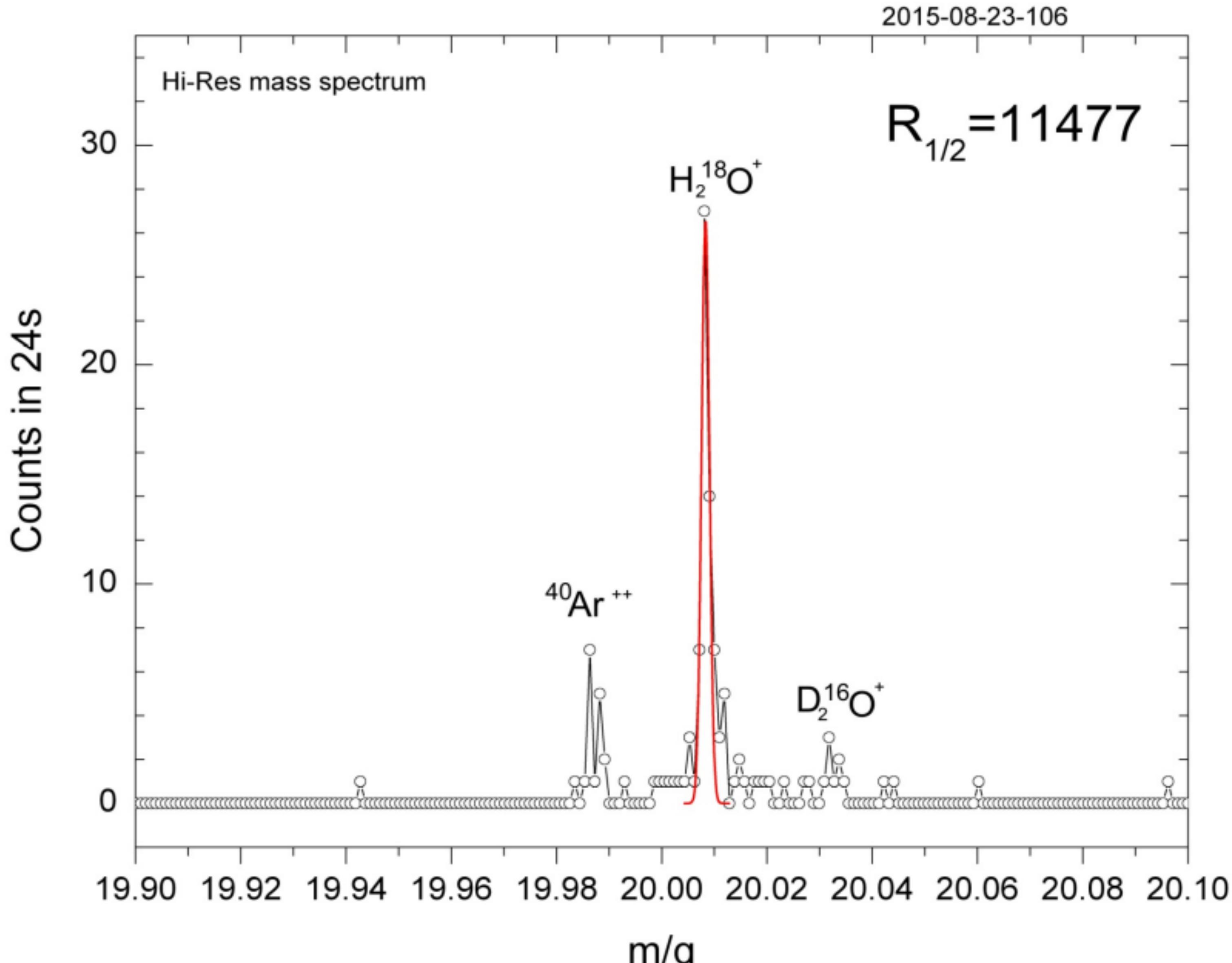
This work was performed at the Jet Propulsion Laboratory (JPL), California Institute of Technology, under a contract with the National Aeronautics and Space Administration (NASA).

Thank you for your attention!

National Aeronautics and Space Administration
Jet Propulsion Laboratory
California Institute of Technology

Questions?

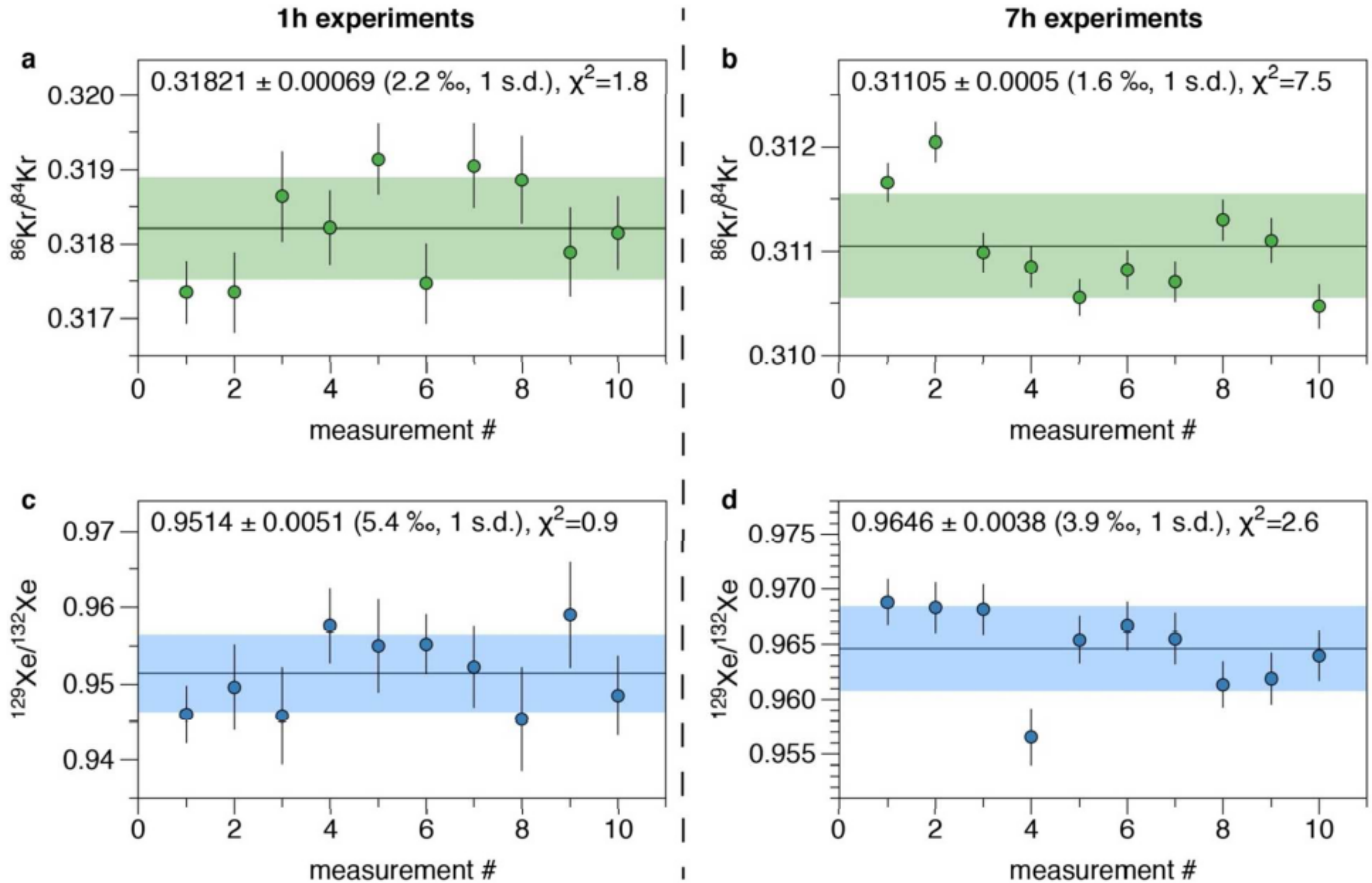
Extra 1: Measured High Resolution Mode



Extra 2 : Expected Performance based on Laboratory

Mass Spectrometer Module	Mass Spectrometer	2.3 kg (CBE + 30%)
	MSIE Electronics	3.94 kg (CBE + 30%)
Total Instrument Mass	6.2 kg (CBE + 30%)	
Sensor Head Dimensions (L x W x H)	15 cm x 15 cm x 15 cm	
MSIE Electronics Dimensions	3 x (1U x 3U) PCBs	
Instrument Field of View	$\pm 10^0$	
Detector Type	Discrete Dynode Electron Multiplier	
Operating Power (W) at 370K trap temperature (CBE +30%)	Peak = 42; Average = 39; Standby = 12	
Data Volume per sec	3.2 kbits (compressed)	
Operating Temp Range	-40 °C to +50 °C	
Survival Temp Range	-200 °C to +130 °C	
Vibration Loads	14g RMS random vibe	
Mass Range	**Low-mass Mode**	0.75 to 10 Th in 2000 channels
	Full-range Mode	0.75 to 230 Th in 2000 channels
Sensitivity	0.01 counts/cm^{-3}/sec	
Mass Resolution (FWHM)	$m/\Delta m \geq$ 1000 @ mass 0.75 to 230	
Dynamic Range	per second: 10^5	per 10 seconds = 10^8
Background Signal Rates — **Day Time (after 1 lunar day bakeout)**	noble gases ≤ 2 counts/sec CO, N_2, CH_4, CO_2 ≤ 5 counts/sec SO_2, Organics: ≤ 2 counts/sec (variable)	
Background Signal Rates — **Total Noise (dark + radiation)**	1×10^{-4} counts/sec/channel (see pg 1-11)	

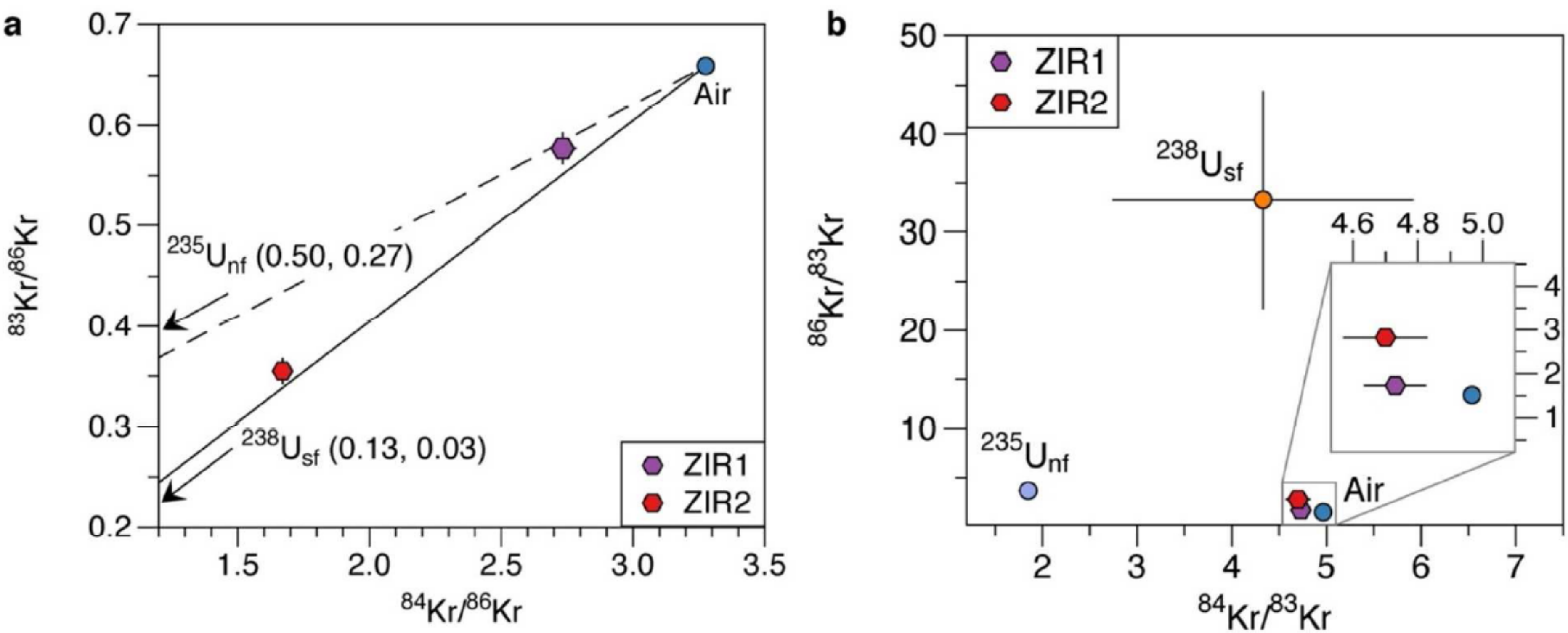
Extra 3: Long-term reproducibility of QIT-MS measurements



Reproducibility of the instrument for 86Kr/84Kr and 129Xe/132Xe ratios characterized through 10 independent measurements of varying duration but set apart by 1hour of idle period; (a) 86Kr/84Kr ratios when 10 measurements were 1hour long; (b) 86Kr/84Kr ratios for 10 measurements each 7hours long; (c) same as (a) but for 129Xe/132Xe ratios; (d) same as (b) but for 129Xe/132Xe; Error bars for each dataset is the 1σ standard deviation.

Extra 4: Isotopic composition of Kr measured in zircons by QIT-MS

The zircon measured in this study is from high-grade metamorphic terrains in northern Sri Lanka. The age of metamorphic resetting of this terrain is ~600 Ma and zircons typically contain high concentration of uranium (1000 ppm) and as a result Xe and Kr isotopes produced by spontaneous fission of 238U have been accumulating in the zircon for the last ~600 Ma. Gas from 600mg of a single zircon megacryst was extracted at Caltech in a resistance furnace in the presence of lithium tetraborate. QITMS is capable of clearly separating both major and minor isotopic ratios in zircons from the those measured in the ambient Air.



Isotopic composition of Kr measured in two different zircons with 1σ error bars; Three-isotope diagrams: (a) showing a clear contribution either from the spontaneous fission of 238U (238Usf) or from the neutron-induced fission of 235U (235Unf), and (b) in another dimensional space showing the distinct isotope composition for 238Usf and 235Unf. Inset is the measured isotope composition in ambient Air.